Water quality and aquatic ecology modelling suite

D-Water Quality

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Particle tracking

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User Manual

D-Particle Tracking

Simulation of mid-field water quality and oil spills, using particle tracking on unstructured grids

User Manual

D-Water Quality

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Disclaimer

D-Particle Tracking currently has a beta status for use on two-dimensional unstructured grids (i.e. in the Delft3D Flexible Mesh Suite or D-HYDRO Suite). While in principle three-dimensional calculations are possible, no support is available.

Currently no GUI is available for D-Particle Tracking in the Delft3D Flexible Mesh Suite and D-HYDRO Suite. This manual is based on the manual for D-Particle Tracking in the Delft3D 4 suite, but the chapters concerning the D-Particle Tracking GUI as part of Delft3D-MENU have been removed. Nevertheless, in the remaining chapters several references to Delft3D-MENU can still be found. These are irrelevant for the use in combination with D-Flow FM. A new manual on using D-Particle Tracking in the Delft3D Flexible Mesh Suite or D-HYDRO Suite will follow at a later stage when D-Particle Tracking will become generally available for unstructured grids.

1 A guide to this manual

1.1 Introduction

In order to make this manual more accessible, a brief description of the contents of each of the chapters will be given here. If you are a novice user of D-Particle Tracking, you are advised to work through the tutorial that is provided in Chapter 4. This should be done in combination with Chapter **??**, where the graphical user interface options are explained in detail.

This document describes the operation of PART within the Delft3D suite.

- **Chapter 2: Introduction to D-Particle Tracking**, a short overview of the program is given together with some specifications of the program package.
- **Chapter 3: Getting started**, the general functionality of the D-Particle Tracking framework is described, together with a brief description of how to start and quit the program.
- **Chapter ??: ??**, provides a detailed description of the Graphical User Interface (PART-GUI).
- **Chapter 4: Tutorial**, provides you with step-by-step instructions to complete a "tracer" and an "oil" tutorial case. Both result in a complete input file and can be executed. Output from the tutorial cases can be compared with the results provided. The emphasis here is to provide practical experience in the use of the module.
- **Chapter 5: Conceptual model**, gives an overview of the modelling concepts used in D-Particle Tracking.
- **Chapter 6: Algorithmic implementation**, describes the algorithms for the advection and dispersion schemes.
- **References**, provides the references used in this manual.
- **Appendix A: Input files D-Particle Tracking**, a description of the ASCII input file (generated by PART-GUI) is given. The ASCII input file can be edited by advanced users who want to apply functionalities that are not (yet) supported by the GUI.

1.2 Manual version and revisions

A manual applies to a certain release of the related numerical program. This manual, version 3.00, applies to D-Particle Tracking version 7.0, and PART-GUI version 2.32.00.

1.3 Typographical conventions

Throughout this manual, the following conventions help you to distinguish between different styles of text used to describe various aspects of the graphical user interface.

Example	Description
Module **Project**	Title of a window or a sub-window are in given in **bold**. Sub-windows are displayed in the **Module** window and cannot be moved. Windows can be moved independently from the **Module** window, such as the **Visualisation Area** window.

Example	Description
Save	Item from a menu, title of a push button or the name of a user interface input field. Upon selecting this item (click or in some cases double click with the left mouse button on it) a related action will be executed; in most cases it will result in displaying some other (sub-)window. In case of an input field you are supposed to enter input data of the required format and in the required domain.
<\tutorial\wave\swan-curvi> <siu.mdw>	Directory names, filenames, and path names are expressed between angle brackets, <>. For Linux environments a forward slash (/) is used instead of the backward slash (\) for Windows environments.
“27 08 1999”	Data to be typed by you into the input fields are displayed between double quotes. Selections of menu items, option boxes etc. are described as such: for instance ‘select *Save* and go to the next window’.
`delft3d-menu`	Commands to be typed by you are given in the font Courier New, 10 points.
➢	In this User manual, user actions are indicated with this arrow.
[m s^{-1}] [–]	Units are given between square brackets when used next to the formulae. Leaving them out might result in misinterpretation. Most units will be in SI notation. [m AD] stands for ’meter Above Datum’, which denotes a level relative to the vertical reference system in the model.

1.4 Changes with respect to previous versions

Version	Description
3.0	Addition of the "unstructured" grids as used by D-Flow FM Removing the description of the separate coupling program (obsolete, as coupling is done within the hydrodynamic modules).
2.15	Update of Friesian Tidal Inlet tutorial model<∗.mdp> file
2.14	Introduction of the <∗.mdp> file

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Version	Description
2.13	PART v3.72.00 and higher can handle thin dams from FLOW. Thus: In **??** Remark removed to warn that thin dams defined in the FLOW model are not recognised in the PART model. In Chapter 4: data files <com-s33.∗> replaced by <com-f35_part.∗>, file <s33_oil.inp> replaced by <s35_oil.inp>; and <s33_tracer.inp> by <s35_tracer.inp>. Finally, figures updates.
2.12	MENU screens updated. Defining coupling input file and starting the coupling now separate MENU options. Remark added about incorrect interpolation of wind direction if the wind passes the North (0 degrees). Remark added to warn that thin dams defined in the FLOW model are not recognised in the PART model.
2.11	The most urgent change that was implemented in the model was the correction of the entrainment of oil in water. Because emulsification was considered essential for the simulation of the fate of oil, this process was also included. Since interaction of processes are significant, a number of feedback mechanisms were also implemented. After implementation, the changes in the specification of the modified compared with the standard oil module is as follows: ◇ Viscosity is now an input parameter and hence an oil characteristic, whilst the entrainment parameter (C0) is now calculated using a relationship that was derived from published data by Delvigne and Hulsen (1994). ◇ Viscosity is not a fixed parameter but a variable, depending on the evaporation and emulsification. ◇ Dispersion (entrainment) process is now consistent with the ADIOS model and independent of the grid. ◇ Emulsification is implemented in the model. ◇ The emulsification is initiated when the evaporated fraction exceeds a given fraction of the oil (input parameter by the user and oil type dependent). ◇ Emulsification is calculated by the increase in the water content of the oil and affects oil viscosity. ◇ Since emulsification affects oil viscosity, entrainment parameter (C0) is affected by a change in viscosity and the entrainment flux reduces when viscosity increases. ◇ Evaporation now affects oil viscosity and hence oil dispersion (entrainment). Evaporation is implemented using the analytical solution of a first order process. ◇ A volatile fraction can be specified. The non-volatile fraction will not be subject to evaporation.

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Version	Description
2.11	Emulsification affects evaporation by using the water content of the oil as calculated during emulsification. When the water content reaches its defined maximum, evaporation ceases. All variables take account of the age of the particles and are being tracked for each particle individually, thus the processes are applied correctly for continuous discharges or several instantaneous discharges at different times.
2.11	**??**: The use of a Zoom grid is compulsory.
2.00	Improved layout of manual.

2 Introduction to D-Particle Tracking

2.1 Short description of the program functionality

The PART module of Delft3D 4 and its successor Delft3D-FM simulates transport and simple water quality processes by means of a particle tracking method using the (2 or 3-dimensional) flow data from the respective hydrodynamic modules. The tracks are followed in three dimensions over time, whereby a dynamic concentration distribution is obtained by calculating the mass of particles in the model grid cells.

The processes are assumed to be deterministic except for a random displacement of the particle at each time step. The particle tracking method is based on a random-walk method since the simulated behaviour is stochastic and the number of particles is limited (Rubinstein, 1981). (It is worth noting that D-Particle Tracking is the only stochastic model in the whole Delft3D suite.)

Particle tracking allows water quality processes to be described in a detailed spatial pattern, resolving sub-grid concentration distributions. D-Particle Tracking is best suited for studies over the mid-field range (200 m – 15 km) of instantaneous or continuous releases, simulation of a plume (for example oil-spill), and modelling of the transport of substances such as salt, bacteria, rhodamine dye, oil, BOD, or other conservative or decaying chemical substances (following first-order kinetics). For this reason, the D-Particle Tracking module is often referred to as the **Mid-field Water Quality** module.

In D-Particle Tracking, several modules are available, only the first two are described here:

- Tracer module: simulation of conservative or first order decaying substances.
- Oil spill module: simulation of oil spills with floating and dispersed oil fractions.
- Specialised modules, among which agent-based ecological modules.

Physical components

The physical components of the D-Particle Tracking model system include:

- the water system: a lake, estuary, harbour or river, possibly with open boundaries to other water systems. Tidal variations are included.
- discharges due to human activities that may be instantaneous and/or continuous;
- chemical substances like rhodamine dyes, salt, oil or suspended solids;
- time varying wind fields;
- settling and erosion of suspended matter;
- concentration dependent settling velocity.

Releases may be defined as instantaneous releases (e.g. dye releases) or continuous releases (e.g. from sewage outfalls).

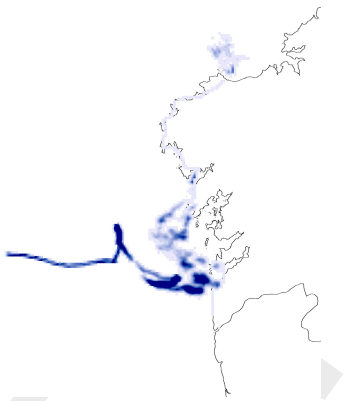

Figure 2.1: *Example of a D-Particle Tracking oil spill simulation*

Physical processes

Physical processes or phenomena that the model was designed to represent are:

- the dynamics of patches close to an outfall location;
- simple first-order decay processes like the decay of several fractions of oil;
- vertical dispersion for well-mixed systems;
- horizontal dispersion due to turbulence. According to turbulence theory this dispersion increases in time.
- the effects of time-varying wind fields on the patches;
- the effects of bottom-friction on the patches;
- the existence of a plume at the outfall (rather than a point-source) by starting the simulation from a circular plume with an estimated or field-measured radius.
- settling of particles, where a concentration dependent settling, subject to a minimum and maximum settling velocity, can be specified;
- transport and fate of spilled oil. Processes that are included in the oil module are: advection of floating oil by wind and currents, dispersion (entrainment in water) of oil induced by wind waves (depending on wind speed and oil characteristics), evaporation of floating oil, emulsification, decay, and sticking of oil to the coastline or seabed. Changes of oil properties (density, viscosity, water content) due to these processes are included in the oil module. Additional advection due to wind drag is implemented in 3D (for 2D the logarithmic profile of the current speed results in a similar wind driven transport), whilst in 3D a deflection angle is included to represent the Coriolis effect of wind induced advection due to waves.
- the model may be started from a known initial distribution of oil, e.g. a remote sensing image of an oil spill.

Applications

The model may be applied to various problems with the physical components, substances and processes described above. However, the time-scale of simulations is usually limited to a few weeks, in order to simulate accurately using a large number of particles. The model is very often applied for plume (outfall) studies with spatial scales of a few kilometres. In such cases, the hydrodynamic grid is often too coarse for other modelling techniques. The particle tracking method is not limited by the spatial resolution of the hydrodynamic database. Thus, detailed outfall studies can be done even within one computational grid cell covering a large area. A costly refinement of the grid in this area is not required.

How does particle modelling work?

The position of every individual particle can be influenced by:

- advection (transport by water flow)
- diffusion/dispersion (a random component)
- settling (including sedimentation/erosion characteristics)

In D-Particle Tracking, every particle is subject to a random displacement. The distance of the displacement depends on the local dispersion and the time step in the model. The direction of the displacement is random. The method used is often referred to as the 'random walk method' or the 'Monte Carlo method'.

The mass of a particle represents the amount of a substance attached to it. The mass of a particle can be influenced by:

- decay rate (first order decay)
- evaporation (of oil).

In D-Particle Tracking, the position of every individual particle (x, y and z co-ordinate) is known from its release until the end of the simulation. The position of a particle does not depend on the grid (size) used and so sub-grid concentration patterns can be calculated.

A release of a substance is distributed over the number of particles specified in the model run. For example, if a dye release of 10 000 particles is used to represent 100 grams of tracer, then each particle represents 0.01 g of tracer. In a continuous release the specified number of particles is distributed over the complete simulation time. That is, if a total number of 10 000 particles are released in 1 day, this is equivalent to 0.116 particles per second. Furthermore, if each particle is assigned 10 g of tracer, this is equivalent to a continuous release of 1.16 g/s.

The concentration of a substance is determined by the number of particles per unit volume. The volume used to calculate the concentrations is defined in one of two ways:

- The hydrodynamic segments (from the Delft3D-FLOW or D-Flow FM computation).
- Segments of a counting grid, the so-called zoom grid, which can be located in any position in the computational domain. The zoom grid defines a regular, rectangular grid in which the rectangles are usually much smaller than the hydrodynamic segments.

The model simply counts the number of particles present in each volume and calculates the corresponding concentration of each substance.

2.2 Specification of the program package

This User Manual describes the use of the Graphical User Interface (PART-GUI) for the computational model D-Particle Tracking of the Delft3D suite. The PART-GUI enables you to input and to retrieve data necessary for preparation and execution of a modelling run.

The manual also describes input and output files generated by PART-GUI and D-Particle Tracking.

2.3 Installing the program

The installation of the Delft3D suite is described in the Installation Manual that is supplied with the software.

2.4 Error checking

The syntax of the input file is checked by the computational core of D-Particle Tracking. Syntax errors cannot occur if you use the PART-GUI. However, if you edit the input files directly, syntax errors may occur and you are responsible for tracing the origin of the error.

The program may stop without an error message on the screen. Error messages are always given in the report file <∗.out> of the simulation. Looking for the word 'ERROR' (capital letters) in this report file can be very useful.

2.5 Particle tracking module within Delft3D

PART-GUI enables you to interact with the mid-field water quality model D-Particle Tracking. The other GUI modules like FLOW-GUI, WAQ-GUI, etc. enable you to interact with other modules in the Delft3D modelling system. These interactions include the input and retrieval of data that is necessary for preparation, execution and post-processing of a modelling run.

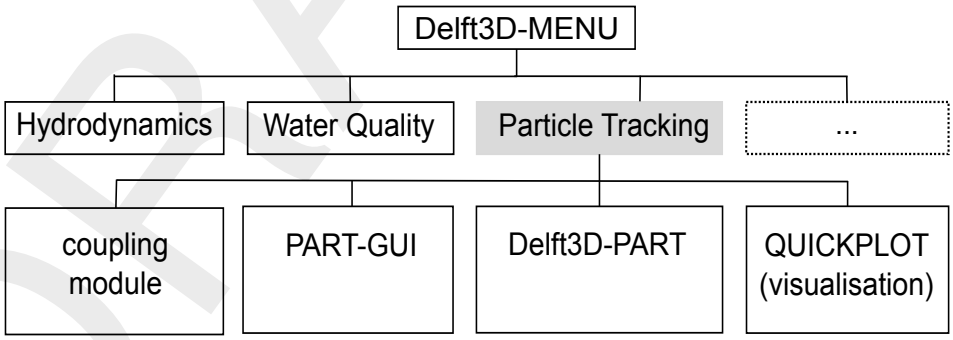

Figure 2.2: *Software architecture around the particle tracking module*

Figure 2.2 shows a part of the Delft3D suite software structure and the location of the **Particle Tracking** module with respect to the other Delft3D modules (e.g. Hydrodynamics, Water Quality, etc.). The most important components in this figure are:

- coupling module (obsolete)
- graphical user interface (PART-GUI)
- particle tracking computational module (D-Particle Tracking)
- Delft3D-QUICKPLOT module for visualisation of results

Descriptions of the other Delft3D 4 and Delft3D FM modules can be found in the associated User Manuals Deltares (2024c,a,b); WAVE UM (2013); GPP UM (2013).

2.6 Input data files

Execution of the D-Particle Tracking computational module depends on the presence of a number of D-Particle Tracking input files. PART-GUI enables you to input data that are necessary for writing an input file and to retrieve data from existing input files. A D-Particle Tracking scenario is defined by the <∗.mdp> file (mdp: Master Definition Part), the corresponding <∗.inp> and the <∗.hyd> file. For each new scenario the files <∗.mdp> and <∗.inp> are created by PART-GUI. The files <∗.mdp> and <∗.inp> are required when opening an existing scenario. The <∗.hyd> file is created by the hydrodynamic modules.

The input data are divided in data groups: Description, Hydrodynamics, Substances, Time Frame, Initial Condition, Numerical Parameters, Instantaneous Releases, Continuous Releases, Process Parameters, Observation Points and Output Options.

Coupling module

Note: The coupling module that was used in the past is obsolete as all necessary files are generated directly via the hydrodynamic modules (Delft3D-FLOW or D-Flow FM).

2.7 Limitations in PART-GUI

In this section the list of (known) limitations of PART-GUI is described. Most of them have to do with a maximum number of substances, observations points etc. Please take them into account while using the PART-GUI.

Note: You need to use the user-interface that comes with Delft3D 4 to set up a model with D-Particle Tracking instead of the user-interface that comes with Delft3D FM, even if you are using a hydrodynamic model that is based on an unstructured grid.

Table 2.1: *Limitations of the PART-GUI*

Number	Description	Value
1	Maximum number of *substances* (oil counts as 3 substances)	90
2	Maximum number of *continuous releases* (note: number of *instantaneous releases* is unlimited)	25
3	Maximum number of columns in (any) GUI table	70
4	Maximum number of oil types (oil counts as “1”)	30
5	Maximum number of time breakpoints in GUI table	1 000
6	Maximum number of layers in case of PLO output	100

3 Getting started

3.1 Starting D-Particle Tracking

Currently no GUI is available for D-Particle Tracking in the Delft3D Flexible Mesh Suite and D-HYDRO Suite. Instead D-Particle Tracking can be started in a command line interface from the Delft3D Flexible Mesh Suite or D-HYDRO Suite start menu.

When the D-Particle Tracking shortcut is selected, a command prompt will open with the following message:

```
D-Particle Tracking - command line interface
This is the command line interface for running D-Particle Tracking models. The path to the run_delpar script has been added to the PATH for easy access.
```

This shortcut adapts the path so the user can easily run D-Particle Tracking. Inside this command prompt you need to navigate to the folder containing the input files. Then using

```
run_delpar.bat <inputfile>
```

a D-Particle Tracking simulation can be run.

4 Tutorial

4.1 Introduction

This tutorial contains two cases which can be run with the D-Particle Tracking module. The purpose of the tutorial is to:

- Give you experience with setting up a D-Particle Tracking simulation, run the simulation and let you understand what D-Particle Tracking can simulate.
- Check the installation of the D-Particle Tracking-software.

This chapter gives both *descriptive* information about the steps to take to set up a D-Particle Tracking simulation and *GUI-operations* to complete each step. The *GUI-operations* are displayed in the text boxes.

4.2 D-Particle Tracking tutorial cases

4.2.1 Tutorial cases

The tutorial contains two applications of 3D simulations with the Delft3D-FLOW 'Friesian Tidal Inlet' schematisation. This schematisation contains 5 layers (aggregated from 10 hydrodynamic layers) and 330 segments per layer.

The applications are (see also Table 4.1):

- A simulation with two conservative tracers. One substance is released at the surface (layer 1) as an instantaneous (or 'dye') release. The other substance is released continuously in the bottom layer of the model (layer 5).
- A simulation for two oil fractions (Ekofisk and Heavy Fuel Oil) that are released instantaneously and as floating substances (a phase of floating oil on the water surface). The radius of the release is calculated with the oil-spill model. Dispersion of the oil is also calculated with the oil-spill model.

Table 4.1: *Specifications of the tutorial cases*

	Tutorial Case Tracer	**Tutorial Case Oil**
Area	'Friesian Tidal Inlet'	'Friesian Tidal Inlet'
Hydrodynamic database	<com-tut_fti_part.hyd> and associated files	<com-tut_fti_part.hyd> and associated files
Type of substance	Tracer(s)	Oil
Substances	'Tracer' 'Tracer con 52'	Ekofisk Oil Heavy Fuel Oil
D-Particle Tracking input file	<fti_tracer.mdp>	<fti_oil.mdp>

4.2.2 Starting D-Particle Tracking

The D-Particle Tracking model framework is started from the Delft3D-MENU as described in chapter 3 (Getting started).

1. STARTING THE DELFT3D-MENU
Create a new directory first ◇ Create a *new directory* somewhere on your hard-disk where you want to store the results of the Particle tracking simulation. ◇ Copy the <com-tut_fti_part.dat> and <com-tut_fti_part.def> files from your <.../tutorial/part/friesian_tidal_inlet/all_flow_output> directory to this freshly created directory. **Start Delft3D** ◇ Start Delft3D-MENU. ◇ Click *Part*. ◇ Click the *Select working directory* button, the *Select working directory* window appears. ◇ Browse to your freshly created directory and enter this directory. ◇ Click *OK* to close the selection of your current working directory.

4.3 Case 1: Tracer

When a suitable hydrodynamic database is available (typically produced via Delft3D-FLOW or D-Flow FM), the input for a PART simulation can be created. Step by step it will be explained how to set up the input for a PART simulation. Each data group will be explained. In this way the input file (<fti_tracer.mdp>) will be created.

Select the *Define input* button in the selection window for **Particle tracking** (see Figure 4.1).

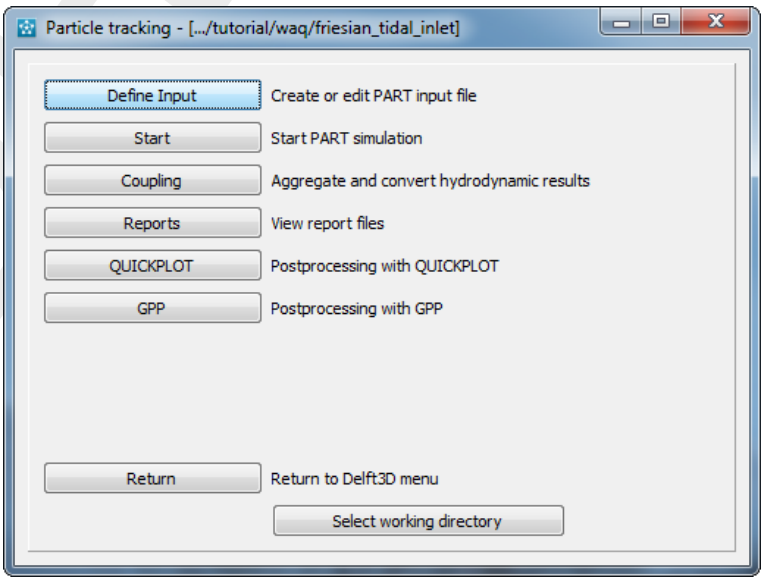

Figure 4.1: *Selection window for* ***Particle tracking***

This will start the PART-GUI (see Figure 4.2). With the GUI, you can input or edit data which are necessary for preparing a D-Particle Tracking scenario (input file). The related data are divided in several data groups. From top to bottom, the following data groups are available: Description, Hydrodynamics, Substances, Time Frame, Initial Condition, Numerical Parameters, Instantaneous Releases, Continuous Releases, Process Parameters, Observation Points and Output Options.

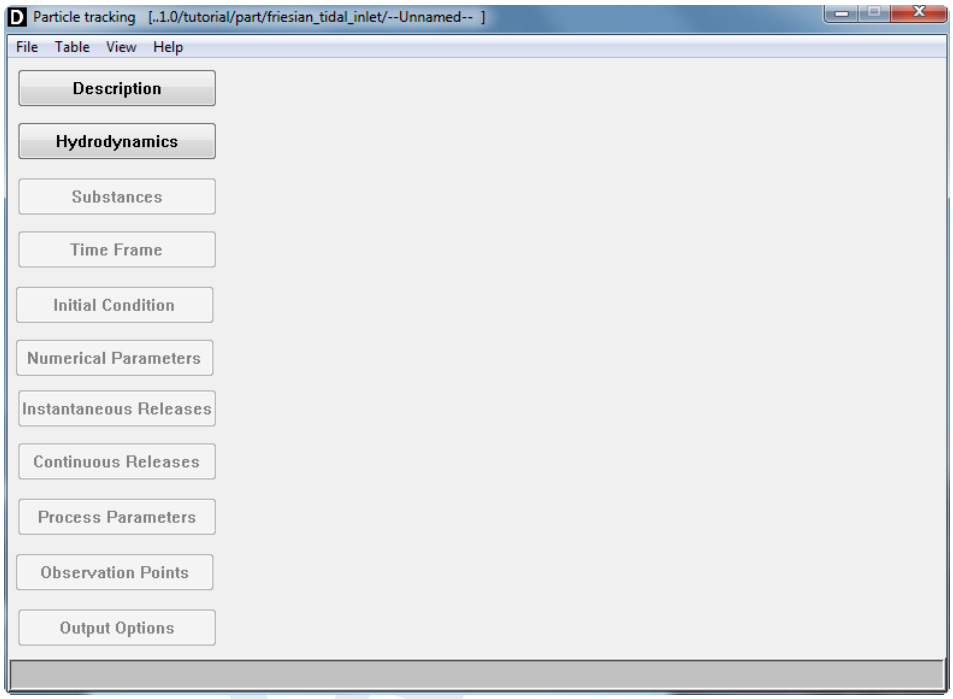

Figure 4.2: *Main window of the PART-GUI*

4.3.1 Description

This data group allows you to add 3 lines of description (meta-information) about the D-Particle Tracking scenario. Specify the 3 lines as in Figure 4.3.

7. DATA GROUP: *description*
In the PART-GUI, select *Description*. Specify the lines of meta data like Figure 4.3.

When finished, you can click on the next data group, *Hydrodynamics*.

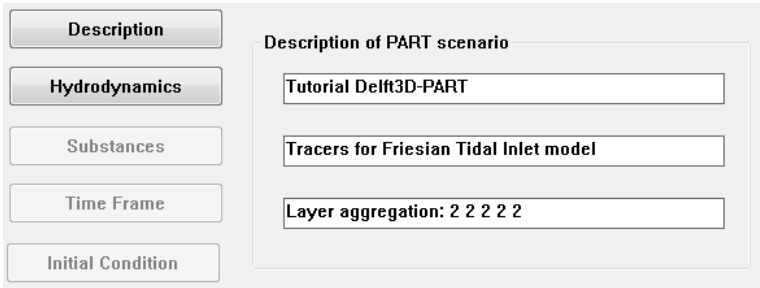

Figure 4.3: *Data Group* Description

4.3.2 Hydrodynamics

Available hydrodynamic results (e.g. <∗.hyd>-files from the coupling module) can be selected in the Data Group *Hydrodynamics*. Press *Select File* to open the **Select hydrodynamics file** window. All the results found in the current working directory are listed; other results can be found by browsing to a different directory. Select the file <com-tut_fti_part.hyd>. The contents is listed in the *Selected hydrodynamic results* frame, Figure 4.4.

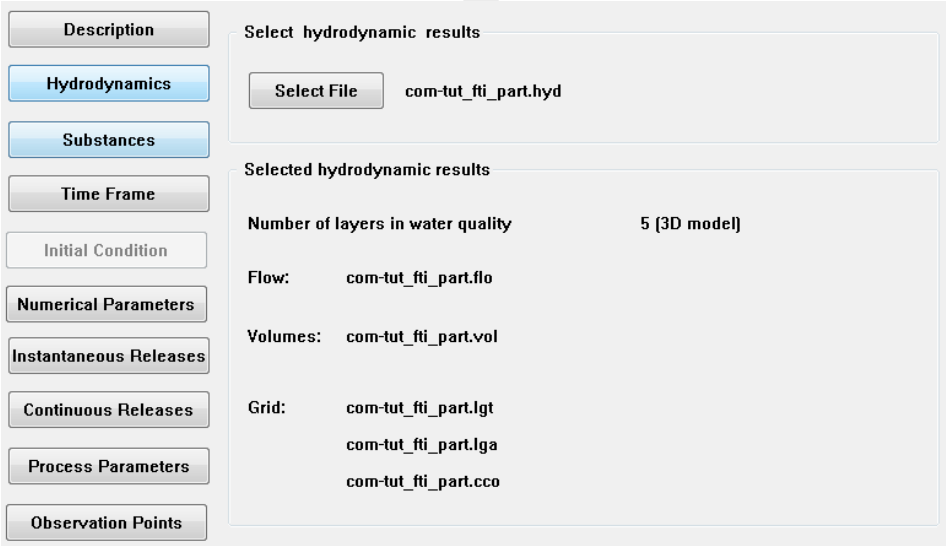

Figure 4.4: *Data Group* Hydrodynamics *showing the selected hydrodynamic results <com-tut_fti_part.hyd>*

8. DATA GROUP: *hydrodynamics*
In the PART-GUI, select *Hydrodynamics*. Press *Select File* and open the <com-tut_fti_part.hyd> file.

4.3.3 Substances

After selection of the Data Group *Substances* the window depicted in Figure 4.5 appears.

Select the *Tracer* radio button and use *Add* to add a second substances. In the list "(New)" appears. Change the name of the substances in:

◇ "Tracer con 52"

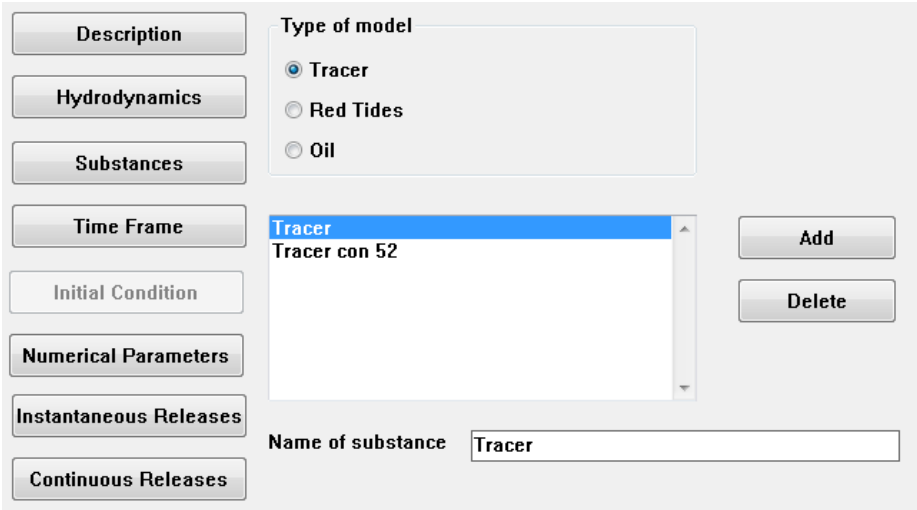

Figure 4.5: *Data group* Substances

9. DATA GROUP: *substances*
In the PART-GUI, select *Substances*. Select radio button *Tracer* in the *Type of model* frame. Change the name in the *Name of substance* edit field into “Tracer”. Click *Add*. Change the name in the *Name of substance* edit field into “Tracer con 52”. Click in the *list box*.

4.3.4 Time frame

Figure 4.6 shows the window corresponding to the *Time Frame* Data Group. The time frame of the hydrodynamic results is given. You can specify the following items:

- Stop time
- Time step

The start time for the water quality calculation cannot be changed. This is equal to the start time of the coupled hydrodynamics.

Set the timings according to Table 4.2.

Table 4.2: *Timers for the Tracer tutorial case*

	Tracer tutorial case
Start time	05/08/1990 12:30:00
Stop time	05/08/1990 20:30:00
Time step for calculation	15 minutes

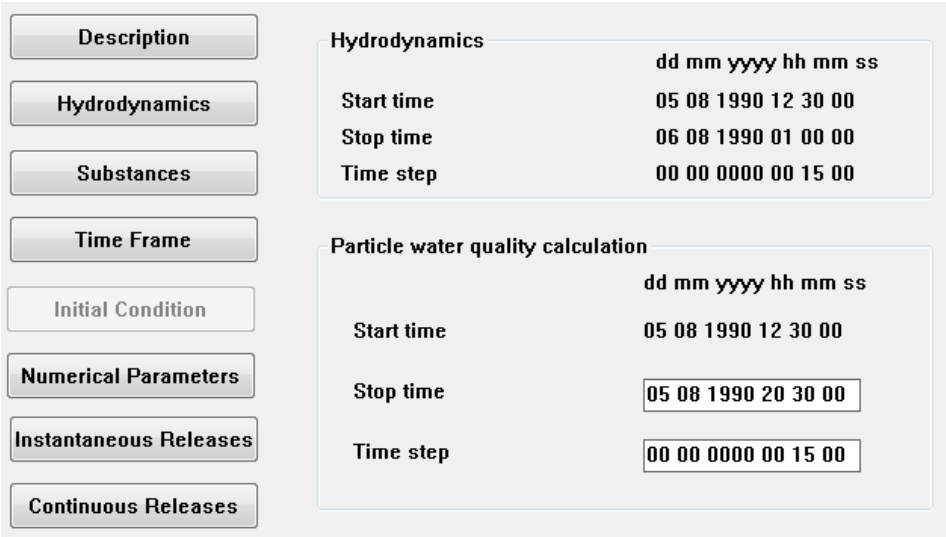

Figure 4.6: *Data Group* Time Frame.

10. DATA GROUP: *time frame*
In the PART-GUI, select *Time Frame*. Specify the *Stop time* edit field: “05 08 1990 20 30 00”. Specify the *Time step* edit field: “00 00 0000 00 15 00”.

4.3.5 Numerical parameters

Figure 4.7 corresponds to the Data Group *Numerical Parameters*. The following numerical parameters can be specified here:

- the number of particles
- vertical diffusion option
- vertical diffusion scaling factor

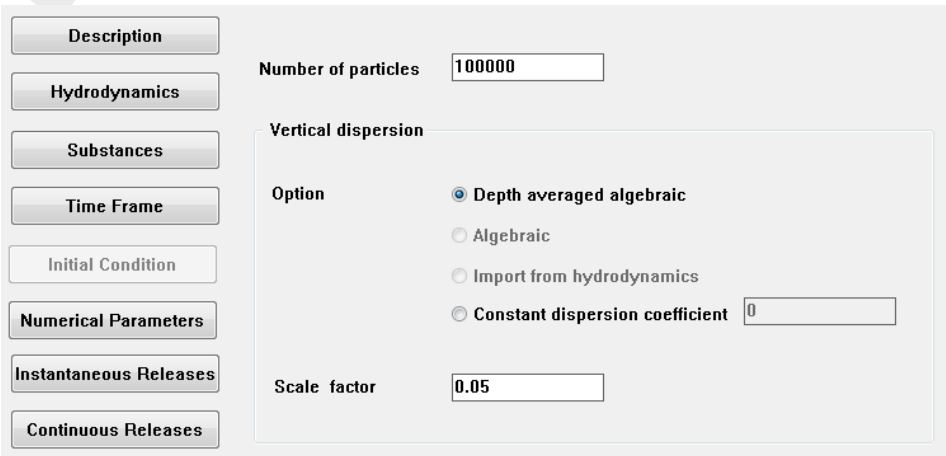

Figure 4.7: *Data Group* Numerical Parameters *after editting*

In this tutorial case, the number of particles is 100 000.

Two vertical diffusion options are available:

- ◇ *Depth averaged algebraic*: the vertical diffusion coefficient is not a function of z, and its integral is approximated by an analytical function. However, it is a function of the (x,y) co-ordinates depending on the local wind stress and bed stress.
- ◇ *Constant dispersion coefficient:* the vertical diffusion coefficient is a constant value for the whole model domain.

The other two options (*Algebraic* and *Import from hydrodynamics)* are expected in the near future, and will have the characteristics:

- ◇ *Algebraic*: coefficient is a function of z and its integral will be approximated.
- ◇ *Import from hydrodynamics:* coefficient is a function of z.

The vertical diffusion scaling factor can be set by you. Its default value is 1, meaning the whole vertical diffusion coefficient is taken in the calculations. For the Tracer tutorial case, the vertical diffusion scaling factor is 0.05.

11. DATA GROUP: *numerical parameters*
In the PART-GUI, select *Numerical Parameters*. Specify “100000” in the *Number of particles* edit field. Specify the “Depth averaged algebraic” radio button in the *Vertical dispersion* frame. Set the *Scale factor* in the *Vertical dispersion* frame to: “0.05”.

4.3.6 Instantaneous releases

An instantaneous discharge of a substance is referred to as a ‘dye release’. In this data group you can prepare (see Figure 4.8): a list of dye releases with corresponding locations (co-ordinates), release radius, particles used (as % of the total number of particles), and a layer number where particles are released (which is 1 for 2D, and can be chosen for 3D calculations).

The location of an instantaneous release can be defined by using point-and-click in the **Visualisation Area**, or the (x,y,z) co-ordinates of the location can be typed in on the main window of this data group. Note that for these locations the particle model does *not* work with grid-cell indices since these are not relevant hereto. The release time and mass of substance released are given in a sub-window. Enter the values in Table 4.3, see Figure 4.8 and Figure 4.9.

Table 4.3: *Details of dye release 1*

Description	Value
release name	dye release 01
location x [m]	193 049
location y [m]	609 122
layer	1
particles (% of total)	50
release radius [m]	0
release time	05/08/1990 12:30:00
substance released	Tracer
amount released [kg]	$1.0 \cdot 10^8$

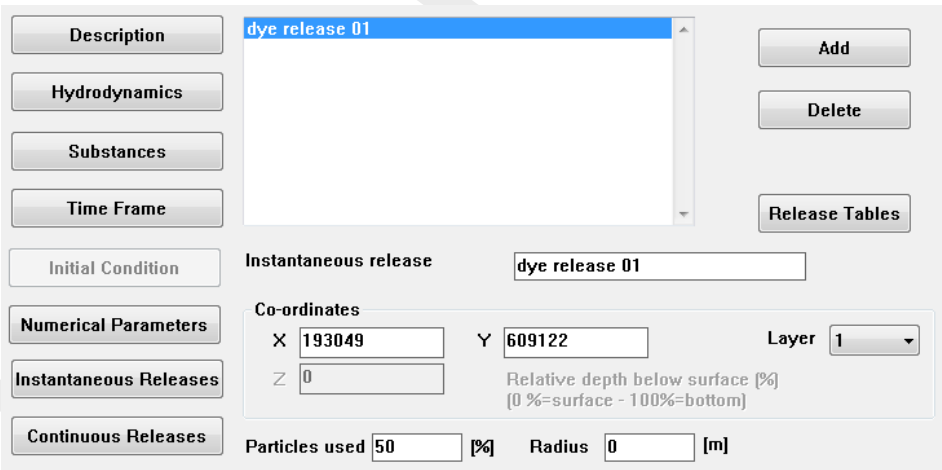

Figure 4.8: *Data Group* Instantaneous Releases

Remarks:

- In a 3D model the release is discharged uniform over the selected layer. The z co-ordinate has no meaning.
- In a 2D model the z co-ordinate is a relative co-ordinate and refers to the relative depth below the water surface (0 % = surface, 100 % = bottom).

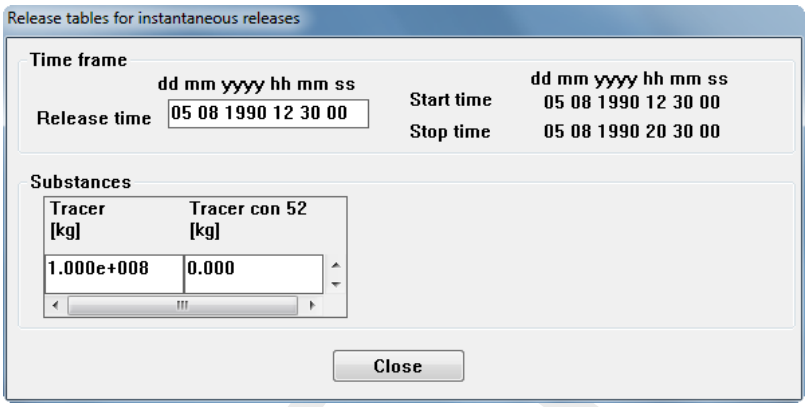

Figure 4.9: Release tables for instantaneous releases *window of a selected instantaneous release*

To use the point-and-click method, do not use *Add*, but select *View* → *Visualisation Area* from the menu bar. Set the *Edit Mode* to *Add*, see Figure 4.10. If not set yet, select *Instantaneous releases* in the *Edit* menu. To define a release at a specific location, move around with the cursor till you reach the specific location and then click with the left mouse. In the main window of the User Interface change the default name '(new)' to 'dye release 01' and set the other characteristics according to Table 4.3.

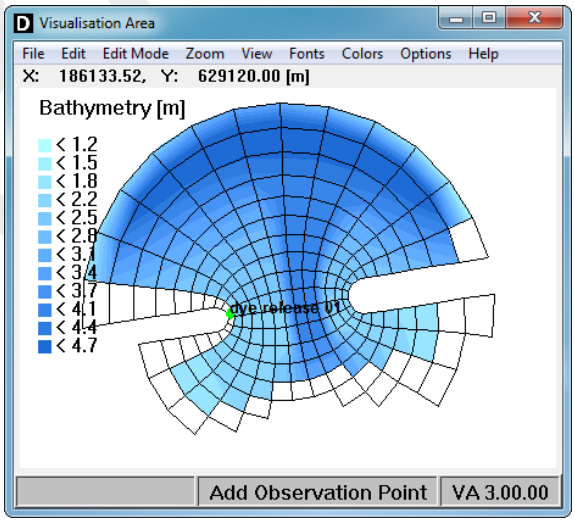

Figure 4.10: *Visualisation Area window*

12. DATA GROUP: *instantaneous releases*
In the PART-GUI, select *Instantaneous Releases*. Click *Add*. Specify "dye release 01" in the *Instantaneous release* edit field. Specify "193049" in the *X* edit field. Specify "609122" in the *Y* edit field. Select layer "1" from the *Layer* drop-down box. Specify "50" in the *Particles used* edit field.

12. DATA GROUP: *instantaneous releases*
Specify “0” in the *Radius* edit field. Select *dye release 1* (from the list) and click *Release Tables*. In the **Release tables for instantaneous releases** window, specify (see Figure 4.9). ◇ “05/08/1990 12:30:00” in the *Release time* edit field (*Time frame* box) ◇ “1.000e+008” in the *Tracer* edit field (*Substances* frame). ◇ Click *Close* to return to the main window.

4.3.7 Continuous releases

In this data group (Figure 4.11 shows the corresponding window) you can prepare a list of continuous releases with corresponding locations, release radius, particles used (as % of the total particles), and a layer number (which is 1 for 2D, and can be chosen for 3D models).

The co-ordinates of the continuous release can be obtained with the **Visualisation Area** or can be typed in on the main window of this data group in (x, y)-co-ordinates. Note that for these locations the particle model does *not* work with grid-cell indices since these are not relevant for particle models. The release rates, stoichiometric coefficients per substance, and scale factor are given in a sub-window.

Table 4.5: *Details of the continuous release*

Description	**Value**
release name	cont. release 01
location x [m]	193567
location y [m]	605871
layer	5
particles (% of total)	50
release radius [m]	0
scale factor	1
release rate [m^3/s]	1.0
substance	Tracer con 52
concentration [kg/m^3]	$1.0 \cdot 10^5$

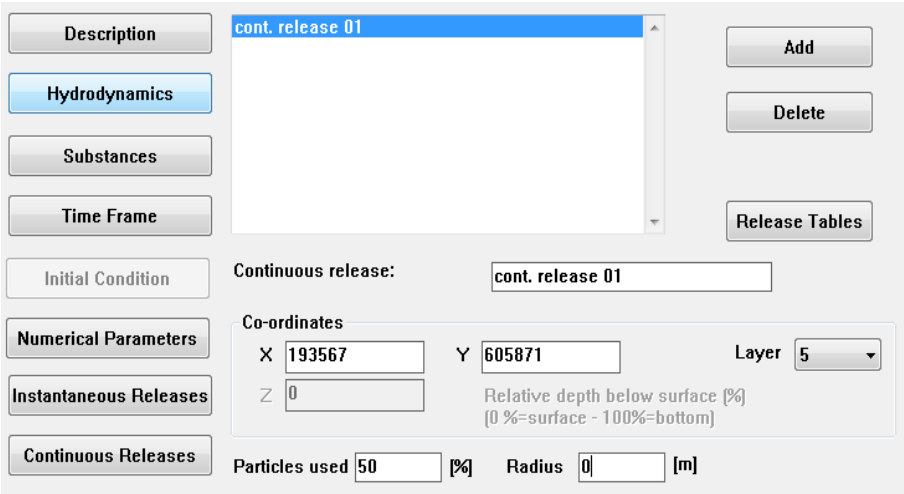

Figure 4.11: *Data Group* Continuous Releases

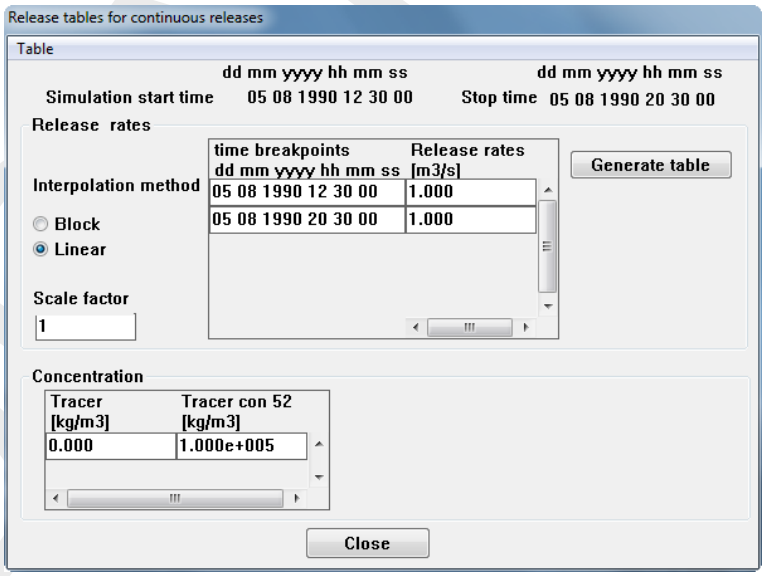

Figure 4.12: Release tables for continuous releases *window of continuous release 1*

13. DATA GROUP: *continuous releases*
In the PART-GUI, select *Continuous releases*. Click *Add*. Specify “continuous release 1” in the *Continuous release* edit field. Specify “193 567” in the *X* edit field. Specify “605 871” in the *Y* edit field. Select layer “5” from the *Layer* drop-down box. Specify “50” in the *Particles used* edit field. Specify “0” in the *Radius* edit field. Select *continuous release 1* (from the list) and click *Release Tables*.

13. DATA GROUP: *continuous releases*
In the **Release tables for continuous releases** window, specify (see Figure 4.12): ◇ Specify in the **first** time breakpoint row: “05 08 1990 12 30 00” in the first column and “1.000” in the second column [m^3/s]. ◇ Specify in the **second** time breakpoint row: “05 08 1990 20 30 00” in the first column and “1.000” in the second column [m^3/s]. ◇ Select interpolation method “linear” (radio button). ◇ Specify *Scale factor*: “1.0”. ◇ “1.000e+005” in the *Tracer con 52* edit field (*Concentration* frame). ◇ Click *Close* to return to the main window.

4.3.8 Process parameters

In the Data Group *Process Parameters* you can define:

- first order decay rates [d^{-1}] for mass decay of substances
- parameters for sedimentation and erosion of particles
- physical parameters (for wind, bed stress and diffusion)
- oil specific parameters (oil model only)

Decay rates

Decay rates are given in a table, per substance and per time breakpoint in units per day. Click *Decay Rates* to display the table (see Figure 4.13).

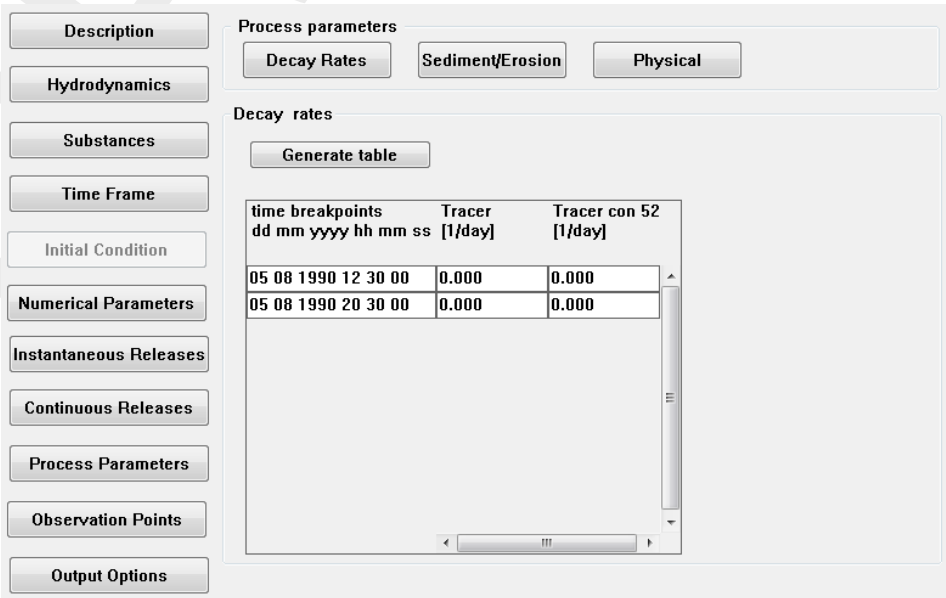

Figure 4.13: *Data Group* Process Parameters *with sub-data group* Decay rates

Sedimentation/Erosion

When clicking *Sedimentation/Erosion*, two additional sub-data groups appear, namely:

- ◇ Constants
- ◇ Settling velocities

First, you must specify if sedimentation and erosion from the bottom is included or excluded (see Figure 4.14). When erosion is included, 3 parameters must be specified for sedimentation and erosion according to Partheniades (1965) and Krone (1962). In the tutorial examples this is not further discussed, since erosion is excluded.

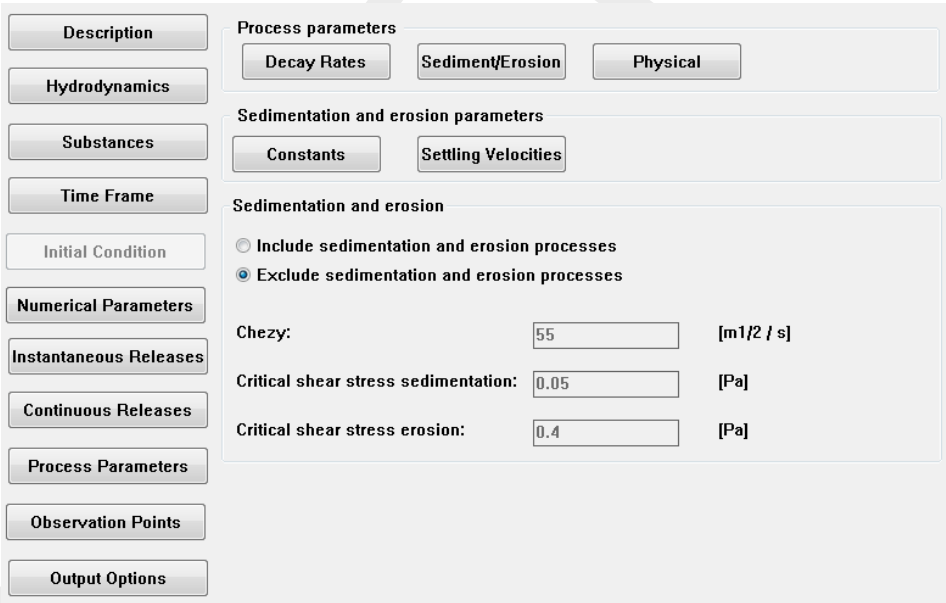

Figure 4.14: *Sub-data group* Sedimentation/erosion – Constants

Settling velocities are given with 6 parameters (two amplitudes, (a_0 and a_1); period (ω), phase (φ), minimum ($v_{\min}$) and maximum ($v_{\max}$) settling velocities) and are also given in tables. Each of the 6 parameters has its own table, per substance and time breakpoint.

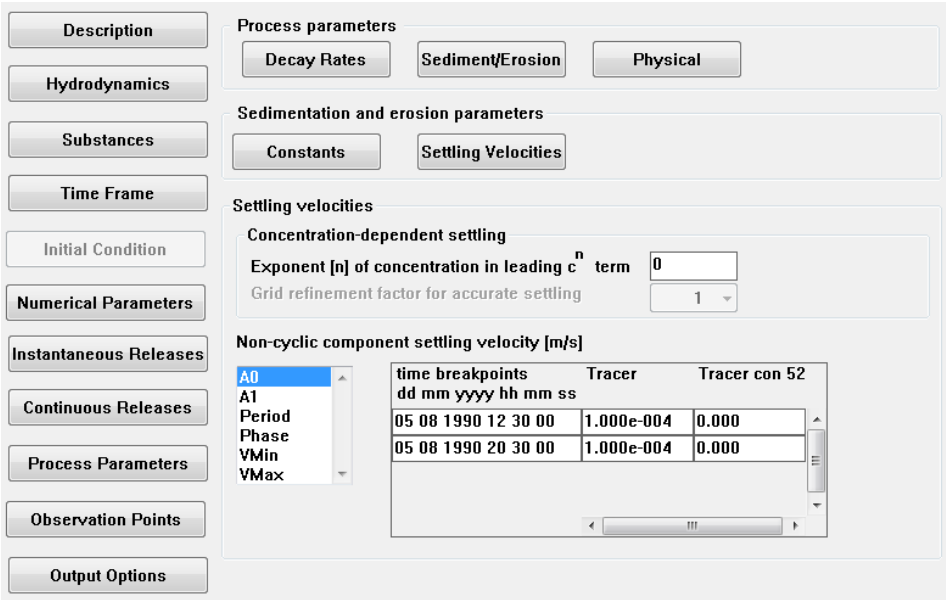

Figure 4.15: *Settling Velocities details (A0 list box selected)*

For this tutorial case, these parameters must be specified as given in Table 4.7.

Table 4.7: *Process parameters*

Description	**Parameter**	**Value**
Decay		No decay
Settling Velocities	A0 [m/s]	$1.0 \cdot 10^{-4}$ (Tacer) 0.0 (Tracer con 52)
	A1 [m/s]	0.0
	period [h]	0.0
	phase [h]	0.0
	$V_{\min}$ [m/s]	-10
	$V_{\max}$ [m/s]	100
Physical Parameters	coefficient a	0.07
	coefficient b	0.7
	roughness [m]	0.002
	wind drag [%]	3.0
	density of water [kg/m^3]	1024.0
	wind speed [m/s]	1
	wind direction [degrees]	270

Physical

So-called physical process parameters contain constants as well as time dependent parameters of wind and horizontal dispersion. See Figure 4.16 and Table 4.7.

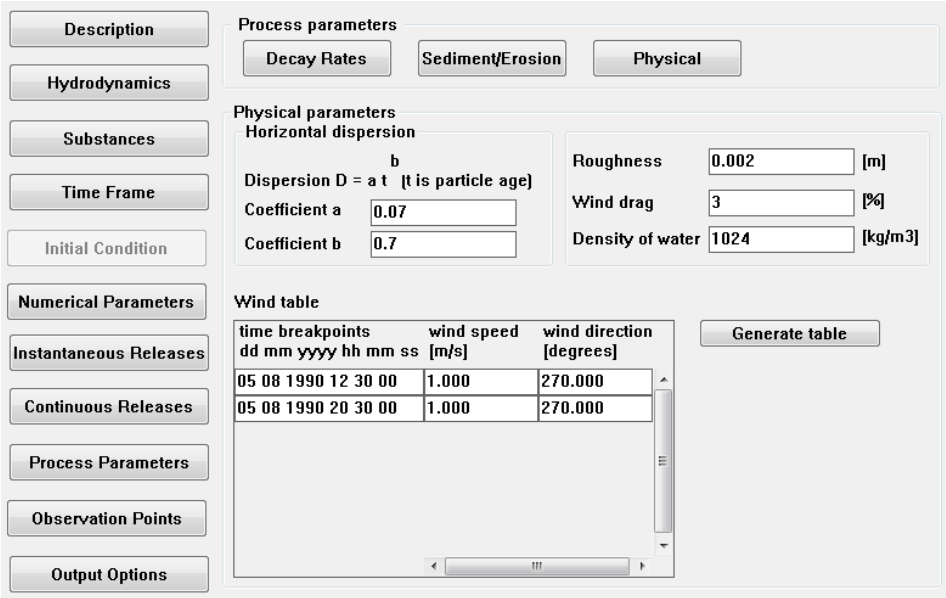

Figure 4.16: *Physical Process parameters*

14. DATA GROUP: *process parameters*
In the PART-GUI, select *Process Parameters*. Click *Decay rates*. Specify the table according to Figure 4.13. Click *Sedimentation/erosion*. Click *Constants*. Select the *Exclude sedimentation and erosion processes* radio button. Click *Settling Velocities*. Specify each item according Table 4.7. Click *Physical*. Specify each item according Table 4.7.

4.3.9 Observation points

To have a time history of results at a single point, observation points can be selected (the corresponding data group window is presented in Figure 4.17). A list of observation points, i.e. their names and their co-ordinates can be given here.

In this tutorial case, a single observation point has been chosen ('waste point') at location:

x = 193 567; y = 605 871

Observation points can also be added with the **Visualisation Area**.

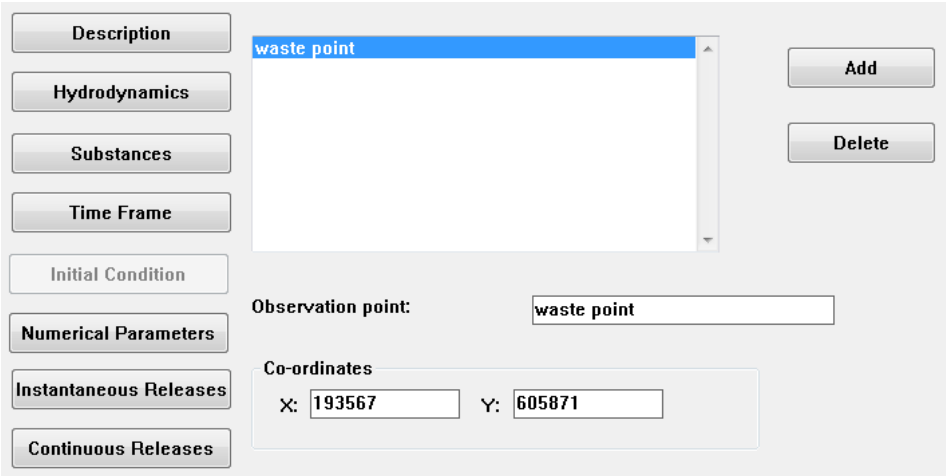

Figure 4.17: *Data Group* Observation Points

15. DATA GROUP: *observation points*
In the PART-GUI, select *Observation points*. Click *Add*. Change the name of the observation point into: “waste point”. Specify “193567” in the *X* edit field. Specify “605871” in the *Y* edit field.

4.3.10 Output options

This data group (see Figure 4.18) contains the time frames for standard output results (history file and map file) and the following additional output options:

- A zoom grid, together with its rectilinear grid dimensions.
- The Zoom Grid Output.

The Zoom Grid Output must be set to specific moments in time using the table displaying the time breakpoints.

(Zoom grid) Grid definition

The zoom grid should be defined in the following way (4 edit fields):

- X: from 185 000 (lower) to 210 000 (upper)
- Y: from 600 000 (lower) to 625 000 (upper)
- Number of cells in both x- and y-direction: 150.

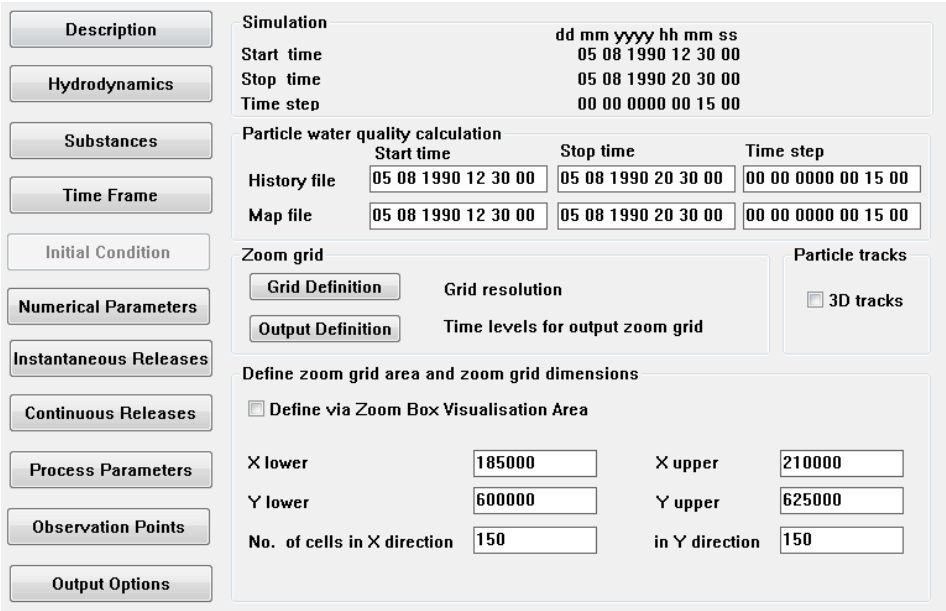

Figure 4.18: *Data Group* Output Options*, with also showing options for* Grid Definition *of the Zoom grid*

16. DATA GROUP: *output options*
In the PART-GUI, select *Output Options*. Change (if necessary) the content of the *Time frame* according Figure 4.18. Click *Grid Definition* in the *Zoom grid* frame. Specify “185000” in the *X lower* edit field. Specify “210000” in the *X upper* edit field. Specify “600000” in the *Y lower* edit field. Specify “625000” in the *Y upper* edit field. Specify “150” in the *Number of cells in X-direction* edit field. Specify “150” in the *Number of cells in Y-direction* edit field. Click *Output Definition*. Specify (using menu-item *Table* → *Insert row*) the number of breakpoints table according Table 4.8.

Table 4.8: *Time breakpoints definition*

time breakpoints **dd mm yyyy hh mm ss**	**recovery factor**
05 08 1990 12 30 00	1.000
05 08 1990 12 45 00	1.000
05 08 1990 13 00 00	1.000
⋮	⋮
05 08 1990 20 15 00	1.000
05 08 1990 20 30 00	1.000

(Zoom grid) Output definition

The tutorial case has 8 time breakpoints for which output is written to this zoom grid. These time breakpoints should be defined (see Figure 4.19). Select a row in the time breakpoints table and select the menu-item *Table* → *Insert row*. Now a row is added to the time breakpoints table. Change the content of the newly added row according to Table 4.8, for this tutorial we use the button *Generate table*.

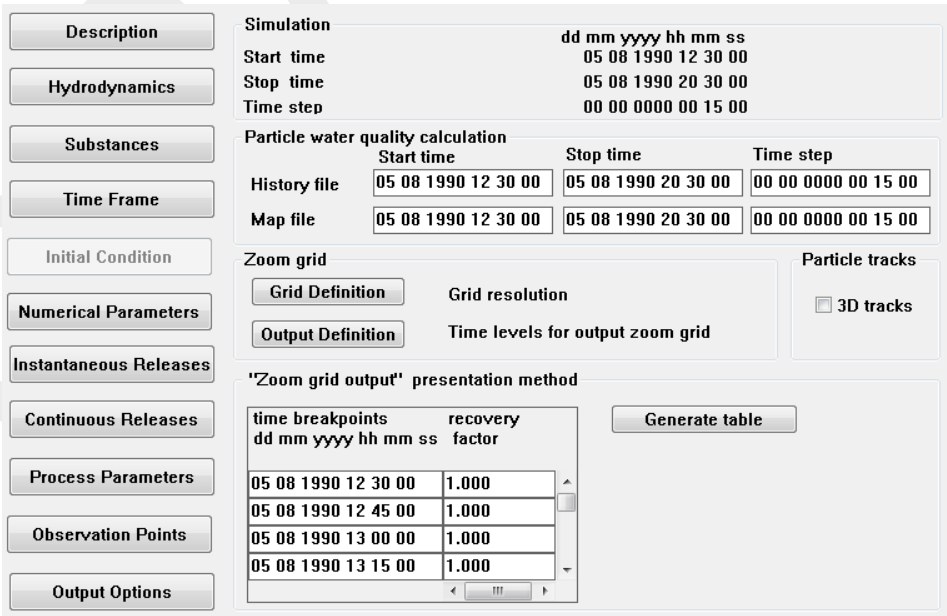

Figure 4.19: *Zoom Grid Output*

4.3.11 Saving the input

By selecting the menu-item *File* → *Save as...* you can specify a file name for your PART simulation. Suggestion is to name it <fti_tracer.mdp>. It will be automatically stored in your current working directory. Select menu-item *File* → *Exit*, ignore the message when you saved your work already. Now your input file is ready and the simulation can take place (see section 4.5).

4.4 Case 2: Oil

We now create the input for a PART-simulation of an oil spill. The hydrodynamic database is the same as in the Tracer tutorial case. Step by step it will be explained how to set-up the input for a PART-simulation (oil module). Each data group will be explained. In this way the input file (<fti_oil.mdp>) will be created.

Select *Define input* in the selection window for **Particle tracking**, see Figure 4.20.

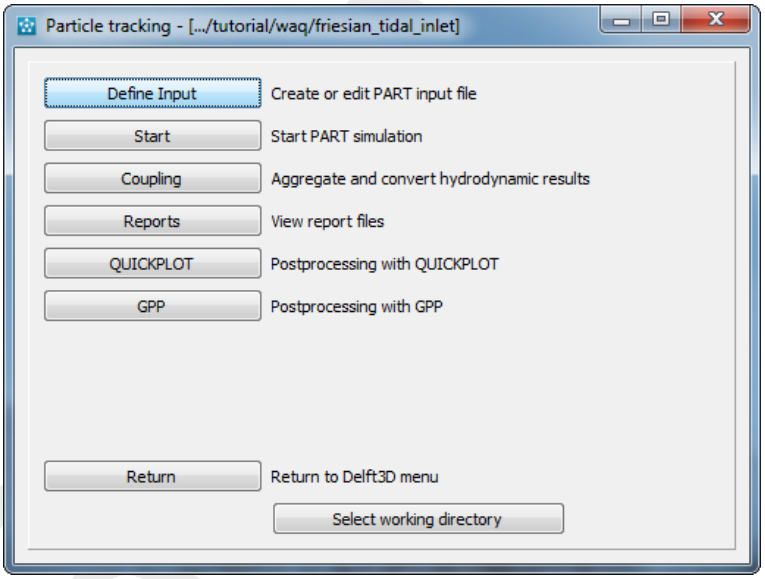

Figure 4.20: *Selection window for* ***Particle tracking***

This will start the PART-GUI (see Figure 4.21). With the GUI you can input or edit data which are necessary for preparing a D-Particle Tracking scenario (input file). The related data are divided in several data groups. From top to bottom, the following data groups are available: Description, Hydrodynamics, Substances, Time Frame, Initial Conditions, Numerical Parameters, Instantaneous Releases, Continuous Releases, Process Parameters, Observation Points and Output Options.

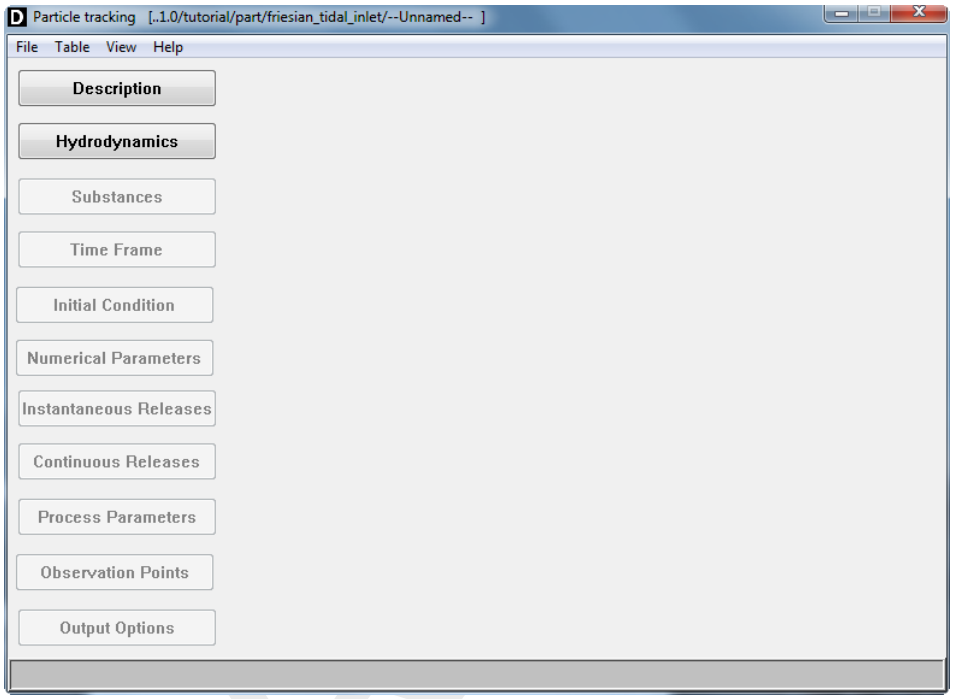

Figure 4.21: *Main window of the PART-GUI*

4.4.1 Description

This data group allows you to add 3 lines of description (meta-information) in a D-Particle Tracking input file. Specify the 3 lines as in Figure 4.3.

1. DATA GROUP: *description*
In the PART-GUI, select *Description*. Specify the lines of metadata like Figure 4.22.

When finished, you can click on the next data group, *Hydrodynamics*.

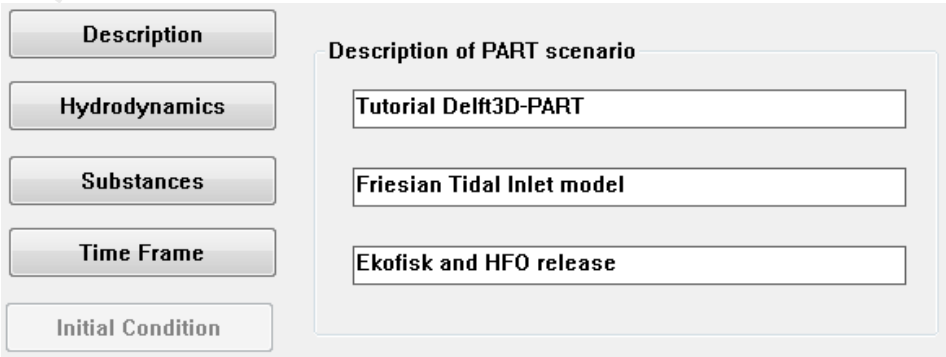

Figure 4.22: *Data Group* Description

4.4.2 Hydrodynamics

Available hydrodynamic results (e.g. <∗.hyd>-files from the **coupling** module) can be selected in the Data Group *Hydrodynamics*. All the results found in the current working directory are listed, whereas other results can be found by browsing to a different directory. The file <com-tut_fti_part.hyd> is already listed in the **Select hydrodynamics file** window.

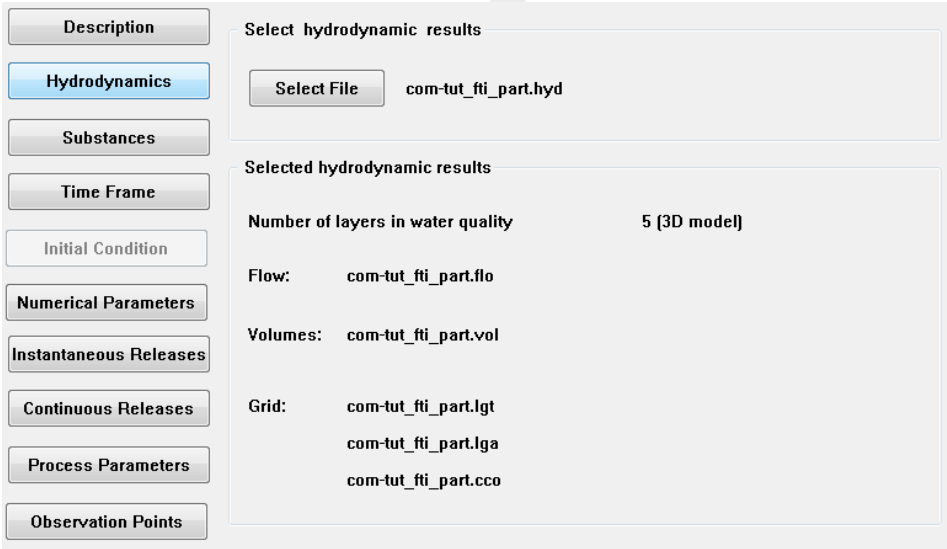

Figure 4.23: *Data Group* Hydrodynamics *showing the selected hydrodynamic results <com-tut_fti_part.hyd>*

2. DATA GROUP: *hydrodynamics*
In the PART-GUI, select *Hydrodynamics* The <com-tut_fti_part.hyd> file is listed in the **Select hydrodynamics file** window.

4.4.3 Substances

After selection of the *Substances* Data Group the window depicted in Figure 4.24 appears.

Select the *Oil* radio button, the oil type “Ekofisk” is immediately available, use the *Add* button to add a second substance. In the list *(new)* appears. Change the name of the substance in:

- ◇ “Heavy Fuel Oil”
- ◇ Click in the *list box*

Note that oil substances are always given in three fractions, namely:

- ◇ Floating oil: oil that is floating as a thin layer on top of the water column,
- ◇ Dispersed oil: oil that is in the water column (‘dissolved’ oil droplets),
- ◇ Sticking oil: oil that (may) stick to land or to the bed, this fraction is no longer transported by water.

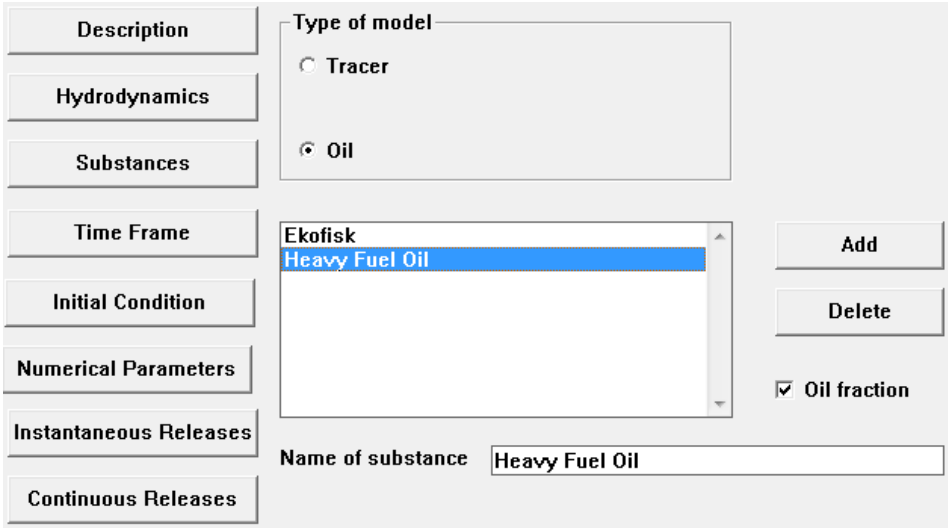

Figure 4.24: *Data Group* Substances

3. DATA GROUP: *substances*
In the PART-GUI, select *Substances*. Select radio button *Oil* in the *Type of model* frame. Change name in the *Name of substance* edit field into “Ekofisk”. Click *Add*. Change name in the *Name of substance* edit field into “Heavy Fuel Oil”. Click in the *list box*.

4.4.4 Time frame

Figure 4.25 shows the window corresponding to the *Time Frame* Data Group. The time frame of the hydrodynamic results is given. You can specify the following items:

- ◇ Stop time
- ◇ Time step

The start time for the water quality calculation cannot be changed. This is equal to the start time of hydrodynamic calculation (after coupling).

Table 4.9: *Timers for the Oil tutorial case*

	Oil tutorial case
Start time	05/08/1990 12:30:00
Stop time	05/08/1990 20:30:00
Time step for calculation	15 minutes

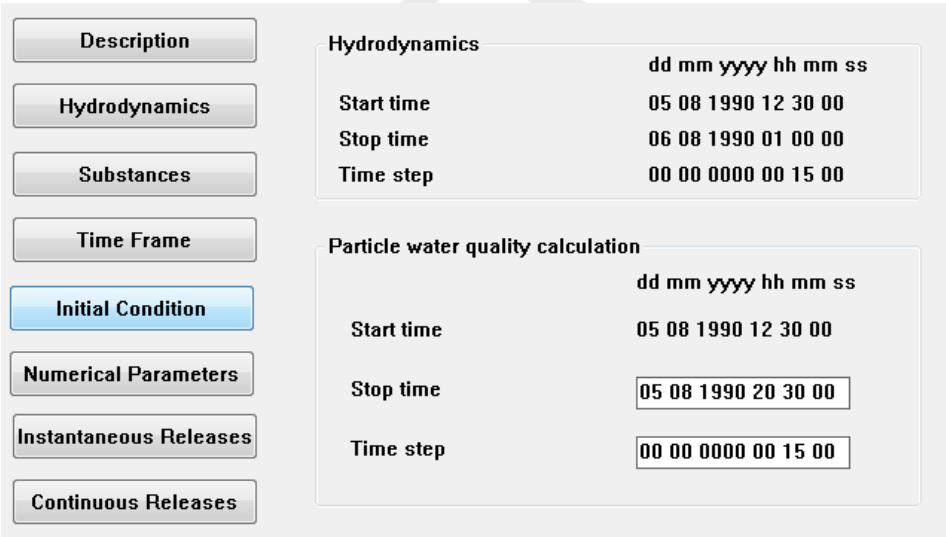

Figure 4.25: *Data Group* Time Frame

4. DATA GROUP: *time frame*
In the PART-GUI, select *Time Frame*. Specify the *Stop time* edit field: “05 08 1990 20 30 00”. Specify the *Time step* edit field: “00 00 0000 00 15 00”.

4.4.5 Initial condition

In this Data Group you select whether or not you want to specify the extent of initial oil patches, by selecting an initial patch file. The file specifies the extent, the amount of oil for each patch and the number of particles to represent each patch of oil. The number of particles specified here are in **addition** to those specified in the *Numerical Parameters* Data Group. The format of the initial condition file is specified in section A.6.

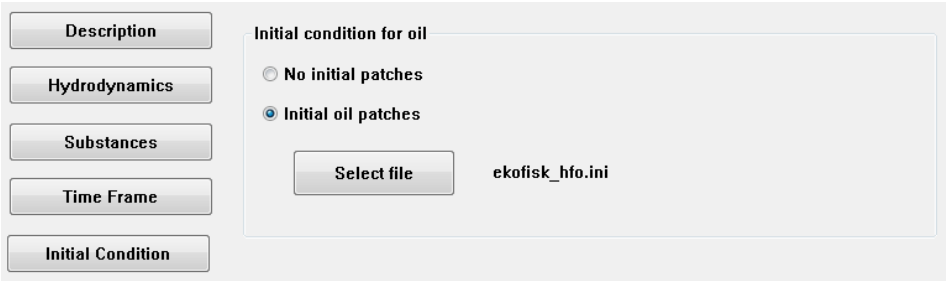

Figure 4.26: *Data Group* Initial Condition

Press *Select file* to open the file with initial patches, see Figure 4.27.

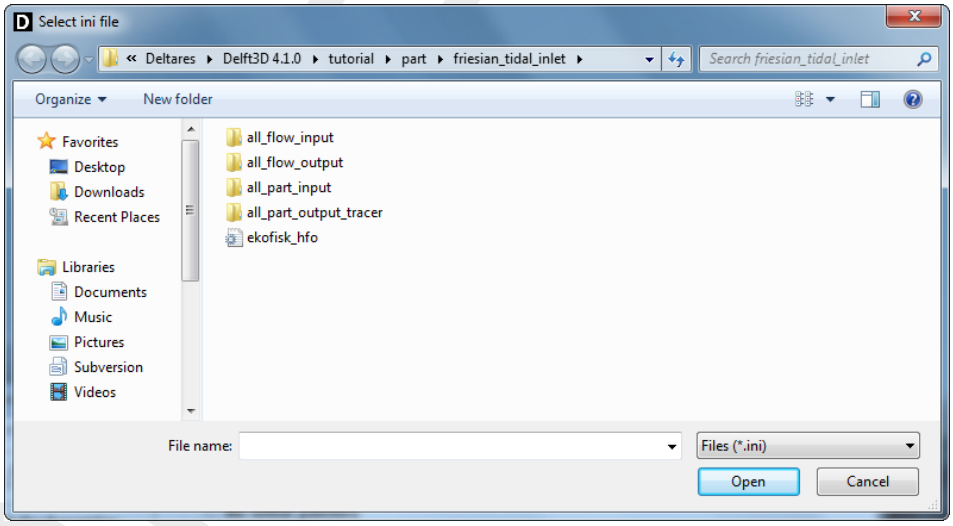

Figure 4.27: *Selection window for the initial conditions file*

5. DATA GROUP: *Initial Condition*
In the PART-GUI, select *Initial Conditions*. Select radio button *Initial oil patches*. Press the *Select file* button. Select file <ekofisk_hfo.ini>. Click *Open*.

4.4.6 Numerical parameters

Figure 4.28 corresponds to the *Numerical Parameters* Data Group. The following numerical parameters can be set here:

- number of particles
- vertical dispersion option
- vertical dispersion scaling factor

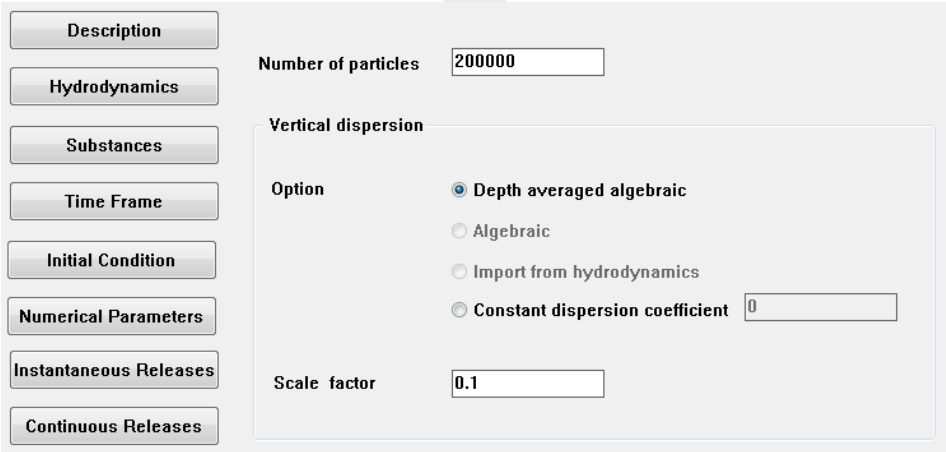

Figure 4.28: *Data Group* Numerical Parameters

In this tutorial case, the number of particles is 200 000.

Two vertical dispersion options are available:

- *Depth averaged algebraic:* the vertical dispersion coefficient is not a function of z, and its integral is approximated by an analytical function. However, it is a function of the (x, y) co-ordinates depending on the local wind stress and bed stress.
- *Constant dispersion coefficient:* the vertical dispersion coefficient is a constant for the whole model domain.

The other two options (*Algebraic* and *Import from hydrodynamics*) are expected in the future, and will have the characteristics:

- *Algebraic*: coefficient is a function of z and its integral will be approximated.
- *Import from hydrodynamics*: coefficient is a function of z.

The vertical dispersion scaling factor can be set by you. Its default value is 1, meaning the whole vertical dispersion coefficient is taken in the calculations. For the Oil tutorial case, the vertical dispersion scaling factor is 0.1.

6. DATA GROUP: *numerical parameters*
In the PART-GUI, select *Numerical Parameters*. Specify “200000” in the *Number of particles* edit field. Specify the “Depth Averaged algebraic” radio button in the *Vertical dispersion* frame. Set the *Scale factor* in the *Vertical dispersion* frame to: “0.1”.

Table 4.10: *Details of oil releases*

Description	**Value**	
release name	oil patch 1	oil patch 2
location x [m]	193049	193567
location y [m]	609122	605871
particles (% of total)	50	50
release radius [m]	calculated	calculated
release time	05/08/1990 12:30:00	05/08/1990 12:30:00
substance released	Ekofisk	Heavy Fuel Oil
amount released	$1.0 \cdot 10^6$ [kg]	$1.0 \cdot 10^6$ [kg]

4.4.7 Instantaneous releases

In this data group you can prepare (see Figure 4.29): a list of instantaneous releases with corresponding locations (co-ordinates), release radius, particles used (as % of the total number of particles), and a layer number where particles are released (which is 1 for 2D, and can be chosen for 3D calculations).

The co-ordinates of the instantaneous release can be obtained with the **Visualisation Area** by point-and-click. You can also enter in the main window of this data group the (x, y, z) co-ordinates. Note that for these locations, as with all location references in PART, the particle model does *not* work with grid-cell indices since these are not relevant hereto. The release time and mass of substance released are given in a sub-window:

Remark:

◇ The volume can be calculated by dividing the total discharge ($1.0 \cdot 10^6$ kg) by the density (850 kg/m^3 for oil patch 1 and 990 kg/m^3 for oil patch 2, see section 4.4.9).

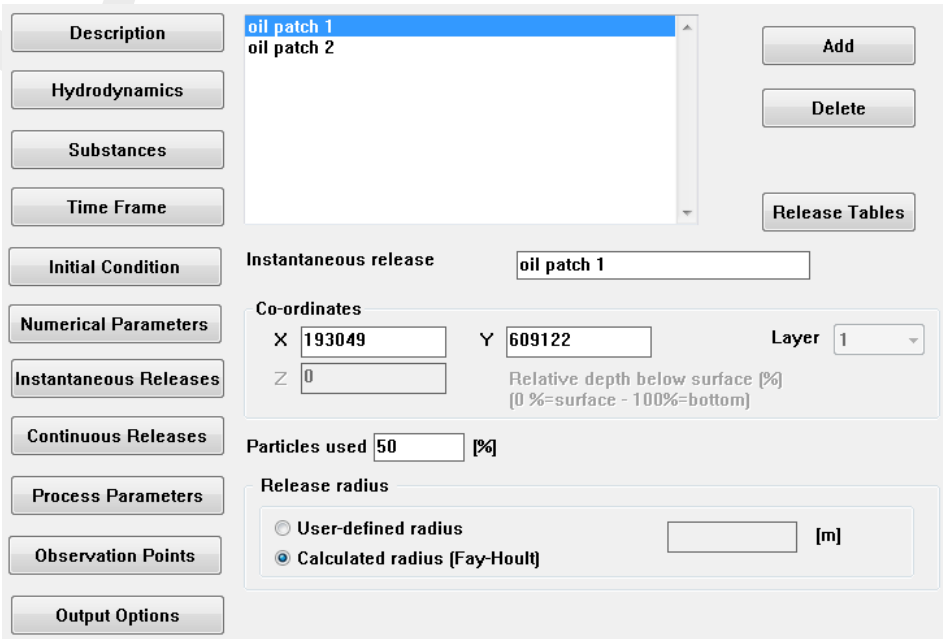

Figure 4.29: *Data Group* Instantaneous Releases

Remark:

◇ Oil can only be released at the water surface (Layer 1, top of that layer). The z-value edit field and Layer drop-down box are disabled.

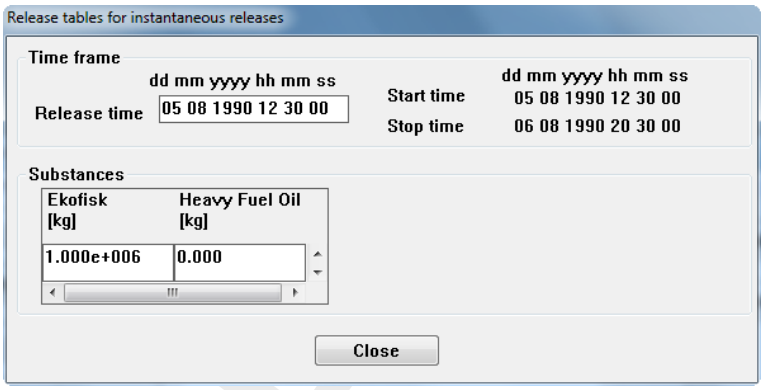

Figure 4.30: Release tables for instantaneous releases *window for oil patch 1*

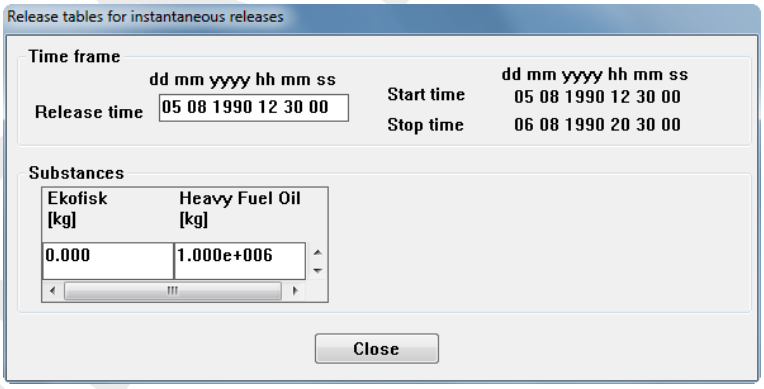

Figure 4.31: Release tables for instantaneous releases *window for oil patch 2*

7. DATA GROUP: *instantaneous releases*
In the PART-GUI, select *Instantaneous Releases*. Click *Add*. Specify “oil patch 1” in the *Instantaneous release* edit field. Specify “193049” in the *X* edit field. Specify “609122” in the *Y* edit field. Specify “50” in the *Particles used* edit field. Select radio button *Calculated radius*. Click *Add* (again). Specify “oil patch 2” in the *Instantaneous release* edit field. Specify “193567” in the *X* edit field. Specify “605871” in the *Y* edit field. Specify “50” in the *Particles used* edit field. Select radio button *Calculated radius*.

7. DATA GROUP: *instantaneous releases*
Select *oil patch 1* (from the list) and click *Release Tables*. In the **Release tables for instantaneous releases** window, specify (see Figure 4.30). ◇ "05/08/1990 12:30:00" in the *Release time* edit field (*Time frame* box). ◇ "1.000e+006" in the *Ekofisk* edit field (*Substances* box). ◇ Click *Close* to return to the main window. Select *oil patch 2* (from the list) and click *Release Tables*. In the **Release tables for instantaneous releases** window, specify (see Figure 4.31): ◇ "05/08/1990 12:30:00" in the *Release time* edit field (*Time frame* box). ◇ "1.000e+006" in the *Heavy Fuel Oil* edit field (*Substances* box). ◇ Click *Close* to return to the main window.

4.4.8 Continuous releases

There are no continuous releases in this tutorial case.

4.4.9 Process parameters

In the Data Group *Process Parameters* (see Figure 4.32) you can define:

- first order decay rates [d^{-1}] for mass decay of substances
- parameters for sedimentation and erosion of particles
- physical parameters (for wind, bed stress and diffusion)
- oil specific parameters (oil model only)

Decay rates

Decay rates are given in a table, per substance and per time breakpoint in units per day. For oil you can specify decay rates per fraction (floating, dispersed, sticked). Click *Decay Rates* to inspect the table. All values should be zero (use the horizontal scroll bar).

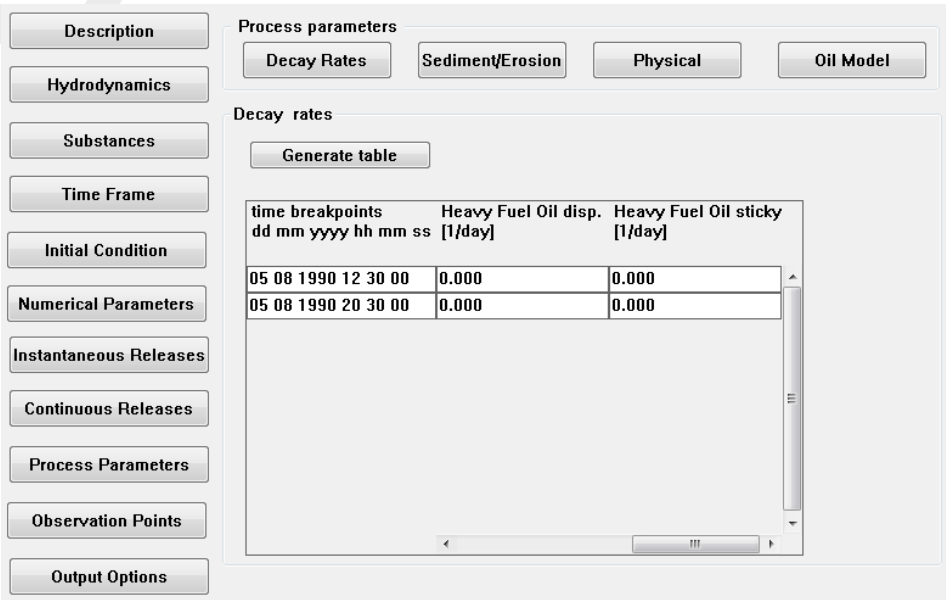

Figure 4.32: *Data Group* Process parameters *with sub-data group* Decay rates

Sedimentation/Erosion

When clicking *Sedimentation/Erosion*, two additional sub-data groups appear, namely:

- ◇ Constants
- ◇ Settling Velocities

First, you must specify if sedimentation or erosion from the bottom is included or excluded (see Figure 4.33). When erosion is included, parameters must be specified for sedimentation and erosion according to Partheniades (1965) and Krone (1962). In the tutorial examples this is not further discussed, since erosion is excluded.

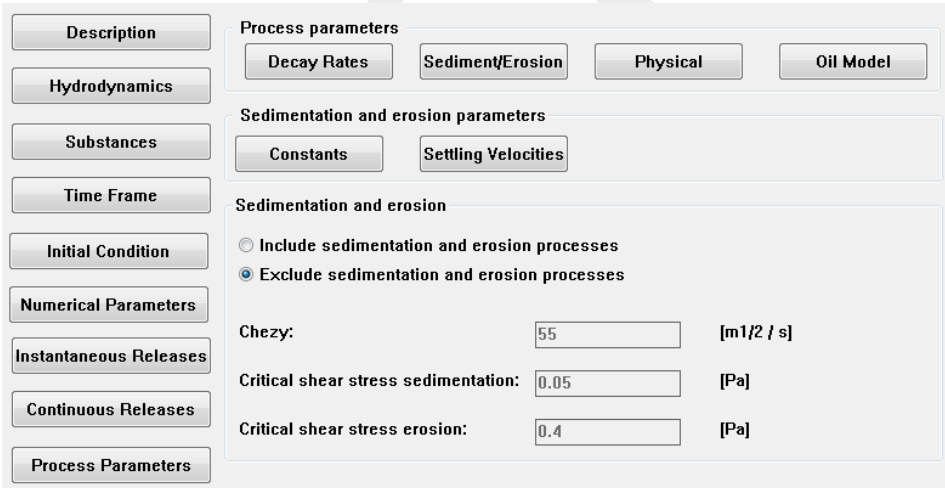

Figure 4.33: *Sub-data group* Sedimentation/Erosion

Settling velocities are given with 6 parameters (two amplitudes, (a_0 and a_1); period (ω), phase (φ), minimum ($v_{\min}$) and maximum ($v_{\max}$) settling velocities), and are also given in tables. Each of the 6 parameters has its own table, per substance and time breakpoint.

Remark:

- ◇ The time breakpoints most be the same for all parameters.

Table 4.12: *Process parameters for Sedimentation and Erosion*

Description	**Parameter**	**Value**
Settling Velocities for	A0 [m/s]	$-1.0 \cdot 10^{-4}$
Ekofisk dispersed and	A1 [m/s]	0.0
HFO dispersed	period [h]	0.0
	phase [h]	0.0
	$V_{\min}$ [m/s]	-10
	$V_{\max}$ [m/s]	100

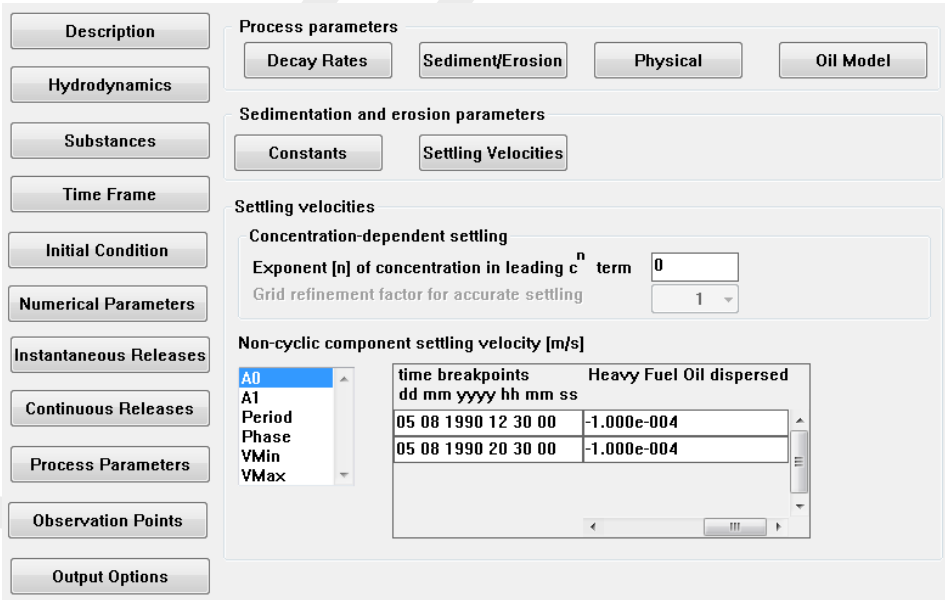

Figure 4.34: *Settling Velocities details (A0 selected in list box)*

For this tutorial case, these parameters must be specified as given in Table 4.14. The negative settling velocity for dispersed oil gives the oil buoyancy.

Physical

So-called physical process parameters contain constants as well as time dependent parameters of wind and horizontal diffusion, see Figure 4.35. These parameters must be specified as given in Table 4.13.

Table 4.13: *Physical process parameters*

Description	Parameter	Value
Physical Parameters	coefficient a	0.07
	coefficient b	0.7
	roughness [m]	0.002
	wind drag (%)	3.0
	density of water [kg/m^3]	1024
	wind speed [m/s]	6
	wind direction [degrees]	270

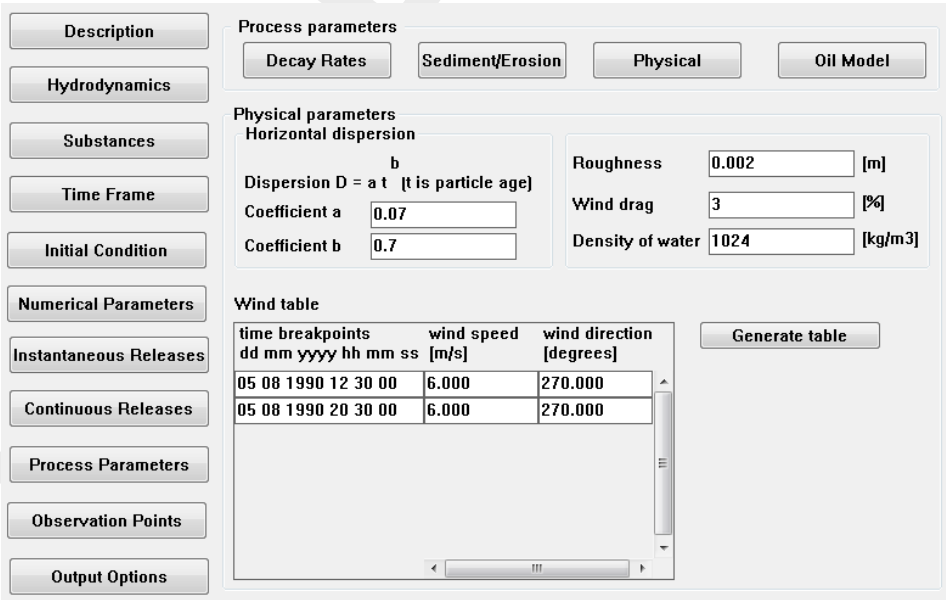

Figure 4.35: *Physical Process parameters*

Oil Model

In this part, specific oil parameters are specified concerning dispersion, evaporation, emulsification, etc., see Figure 4.36. Fill in the values as indicated in Table 4.14.

Table 4.14: *Process parameters for oil*

Description	Parameter	Value	
		Ekofisk	**HFO**
Oil Model	Evaporation per day	0.4	0.05
	Stickyness probability	0.0	0.5
	Volatile fraction	1	0.94
	Emulsification parameter C_1	0	$2 \cdot 10^{-6}$
	Maximum water content	1	0.7
	Fraction at which emulsification starts	1	0.05
	Density	850	990
	Kinematic viscosity	50	1500
	Dispersion (entrainment)	calculated	calculated
	Minimum thickness	0.00005	0.00005
	Deflection angle	0	0

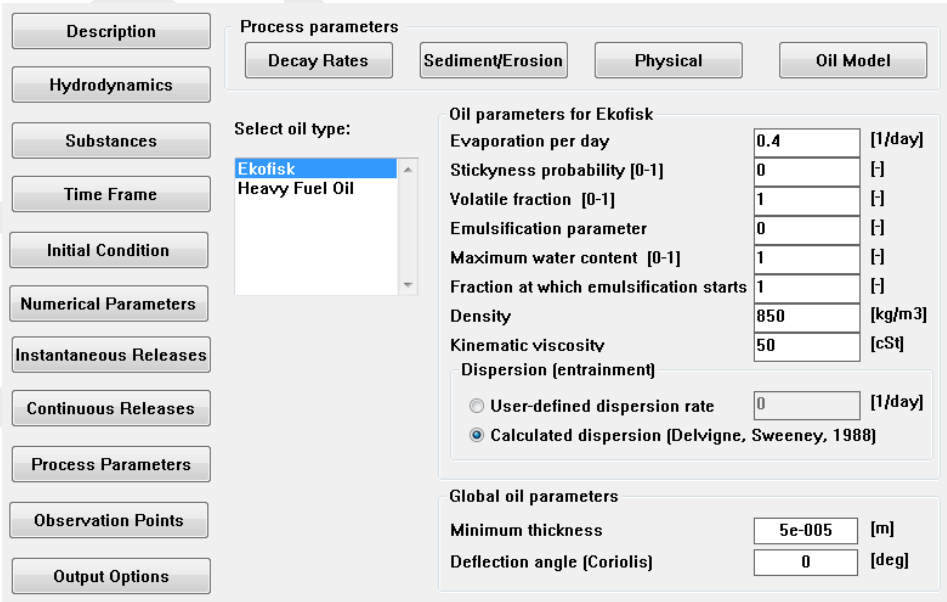

Figure 4.36: *Oil Model specific parameters*

8. DATA GROUP: *process parameters*
In the PART-GUI, select *Process Parameters*. Click *Sedimentation/erosion*. Click *Constants*. Select the *Exclude sedimentation and erosion processes* radio button. Click *Settling Velocities*. Specify each item according to Table 4.12. Click *Physical*. Specify each item according to Table 4.13/Figure 4.35. Click *Oil Model*. Specify each item according to Table 4.14/Figure 4.36.

4.4.10 Observation points

To have a time history of results at a single point, observation points can be selected (the corresponding data group window is presented in Figure 4.17. A list of observation points, i.e. their names and their co-ordinates can be given here.

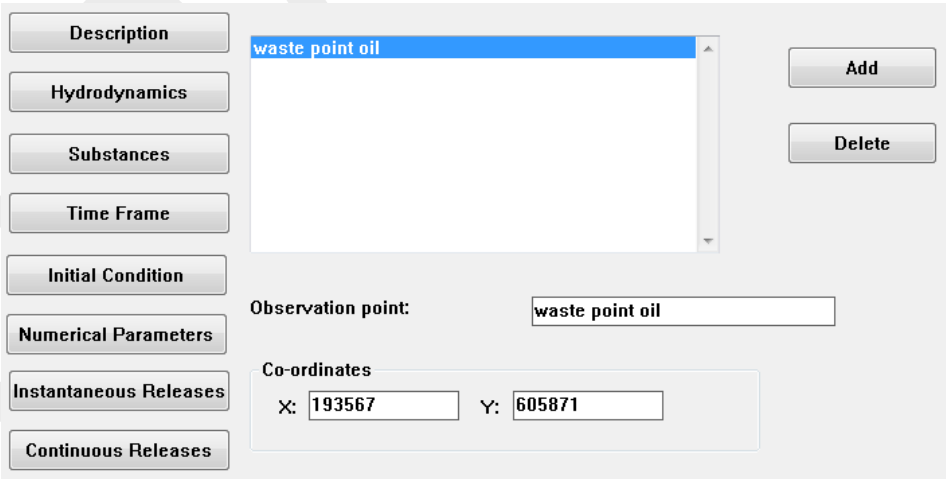

Figure 4.37: *Data Group* Observation Points

In this tutorial case, a single observation point has been chosen ('waste point oil') at location:

x = 193 567; y= 605 871

Observation points can also be added with the **Visualisation Area**.

9. DATA GROUP: *observation points*
In the PART-GUI, select *Observation Points*. Click *Add*. Change the name of the observation point into: “waste point oil”. Specify “193567” in the *X* edit field. Specify “605871” in the *Y* edit field.

4.4.11 Output options

This data group (see Figure 4.38) contains the time frames for standard output results (history file and map file) and additional output mapped on a rectangular zoom grid.

The output to the zoom grid must be set to specific moments in time using the table displaying the time breakpoints.

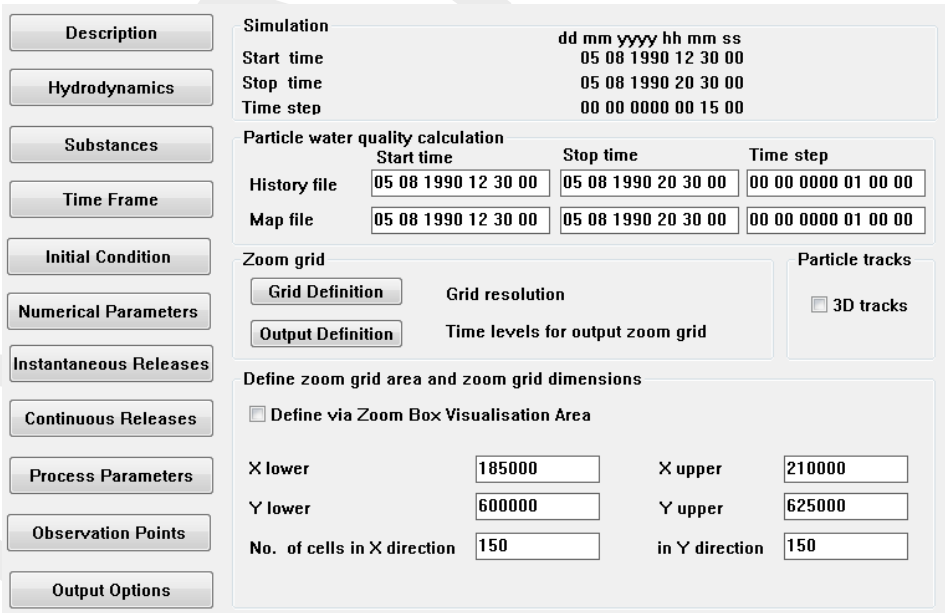

Figure 4.38: *Data Group* Output Options*, also showing options for* Definition of Zoom grid

(Zoom grid) Grid definition

The zoom grid should be defined in the following way (4 edit fields):

- X: from 185000 (lower) to 210000 (upper)
- Y: from 600000 (lower) to 625000 (upper)
- Number of cells in x- and y-direction is: 150.

(Zoom grid) Output definition

The tutorial case has 8 time breakpoints for which output is written to this zoom grid. These time breakpoints should be defined (see Figure 4.39). Select a row in the time breakpoints table and select the menu-item *Table* → *Insert row*. Now a row is added to the time breakpoints table. Change the content of the newly added row according to Table 4.15, for this tutorial we use the button *Generate table*.

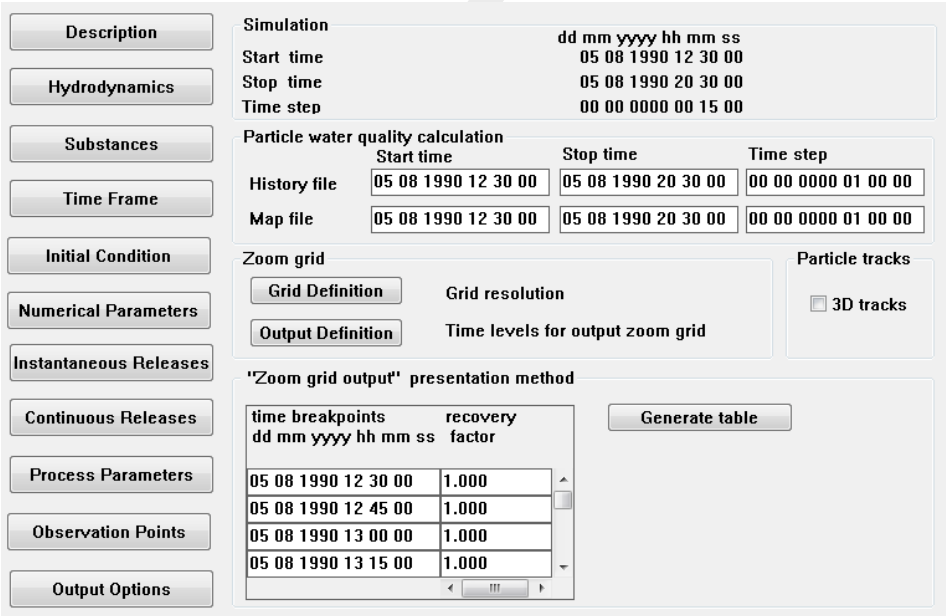

Figure 4.39: *Zoom Grid Output*

Table 4.15: *Time breakpoints definition*

time breakpoints dd mm yyyy hh mm ss	**recovery factor**
05 08 1990 12 30 00	1.000
05 08 1990 12 45 00	1.000
05 08 1990 13 00 00	1.000
⋮	⋮
05 08 1990 20 15 00	1.000
05 08 1990 20 30 00	1.000

4.4.12 Saving the input

By selecting the menu-item *File* → *Save as...* you can specify a file name for your PART simulation. Suggestion is to name it <fti_oil.mdp>. It will be automatically stored in your current working directory. Select menu-item *File* → *Exit* and ignore the message when you already saved your work. Now your input file is ready and the simulation can take place (see section 4.5).

4.5 Executing a scenario

Once you leave the PART-GUI, you will return to the main menu. The calculation can be started by selecting *Start* from the main menu screen (Figure 4.1).

The model will always run with the latest input file that has been opened and saved.

While the model is running, you will see on the screen the hydrodynamic flow and volume records updated, the actual time, and the number of active particles in the calculation. When the calculation is finished, you will again see the main menu of D-Particle Tracking.

When the model stops before the end of simulation without an error message, then check the report file on the word 'ERROR'. Errors in the syntax of the input file must appear directly on the screen in front of you. There should be no errors and no warnings for the two tutorial cases.

4.6 Viewing the report

A report of each model calculation is made, and this can be viewed by selecting *Reports* from the main menu screen. By clicking *Monitoring* and *Select file*, you can browse to the <∗.out> file (∗ = name of scenario). You can scroll through the file to read any error or warning messages for the D-Particle Tracking calculation.

The possible error and warning messages are supposed to be instructive and clear enough for you to make the necessary corrections. Look for the words 'ERROR' and 'WARNING' (capital letters). There should be no errors and no warnings for the two tutorial cases.

4.7 Viewing the results

To view output of a PART simulation, the Delft3D-QUICKPLOT program is used. By selecting *QUICKPLOT* in the selection window for **Particle tracking** (Figure 4.1), *QUICKPLOT* starts.

Remarks:

- ◇ The 'tracer' plot can only be viewed if you have finished the tutorial Tracer case.
- ◇ The 'oil' plot can only be viewed if you have finished the tutorial Oil case.

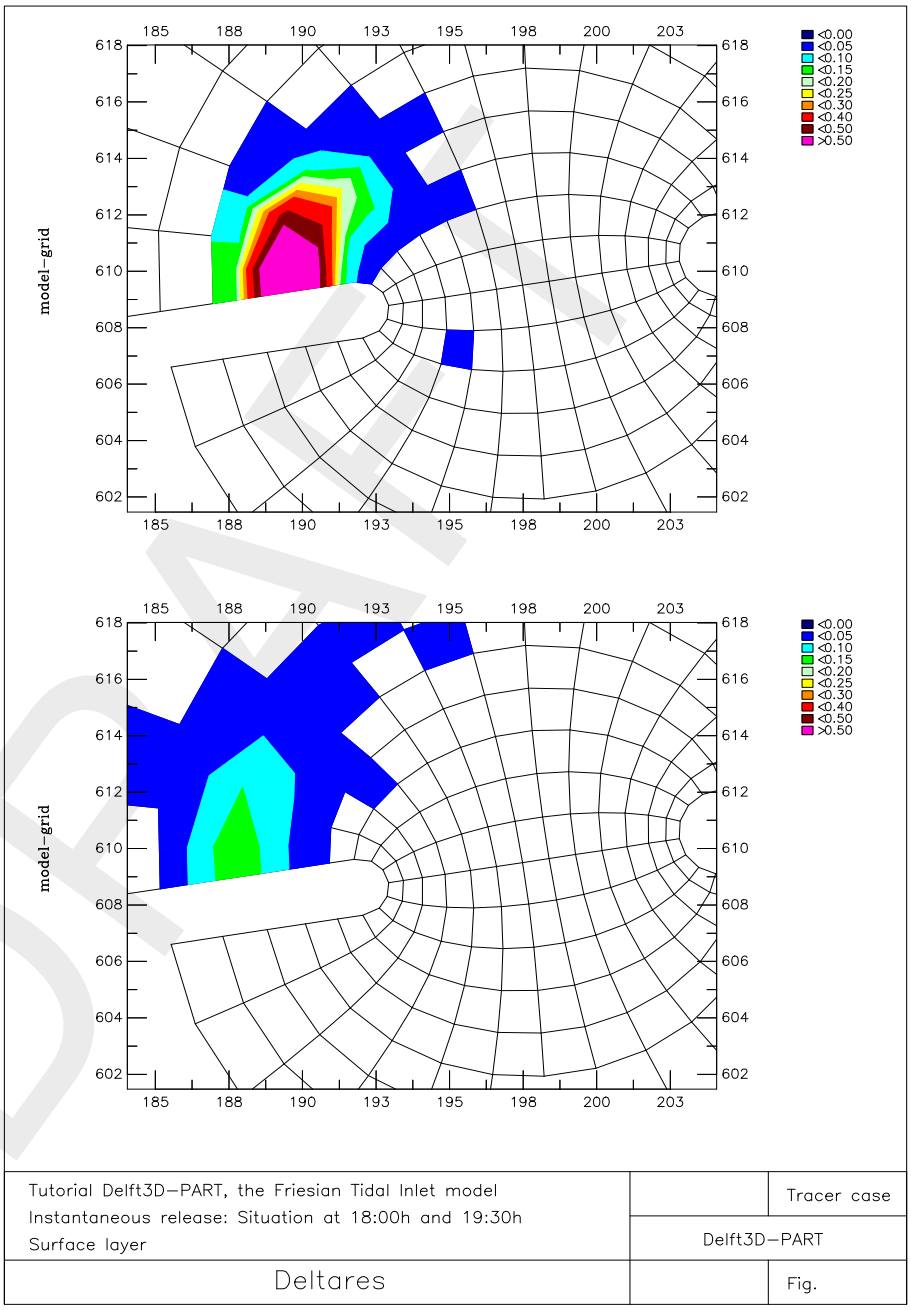

Figure 4.40: *Tracer Case: Instantaneous release: situation at 18:00 hrs (upper) and 19:30 hrs (lower) in the surface layer*

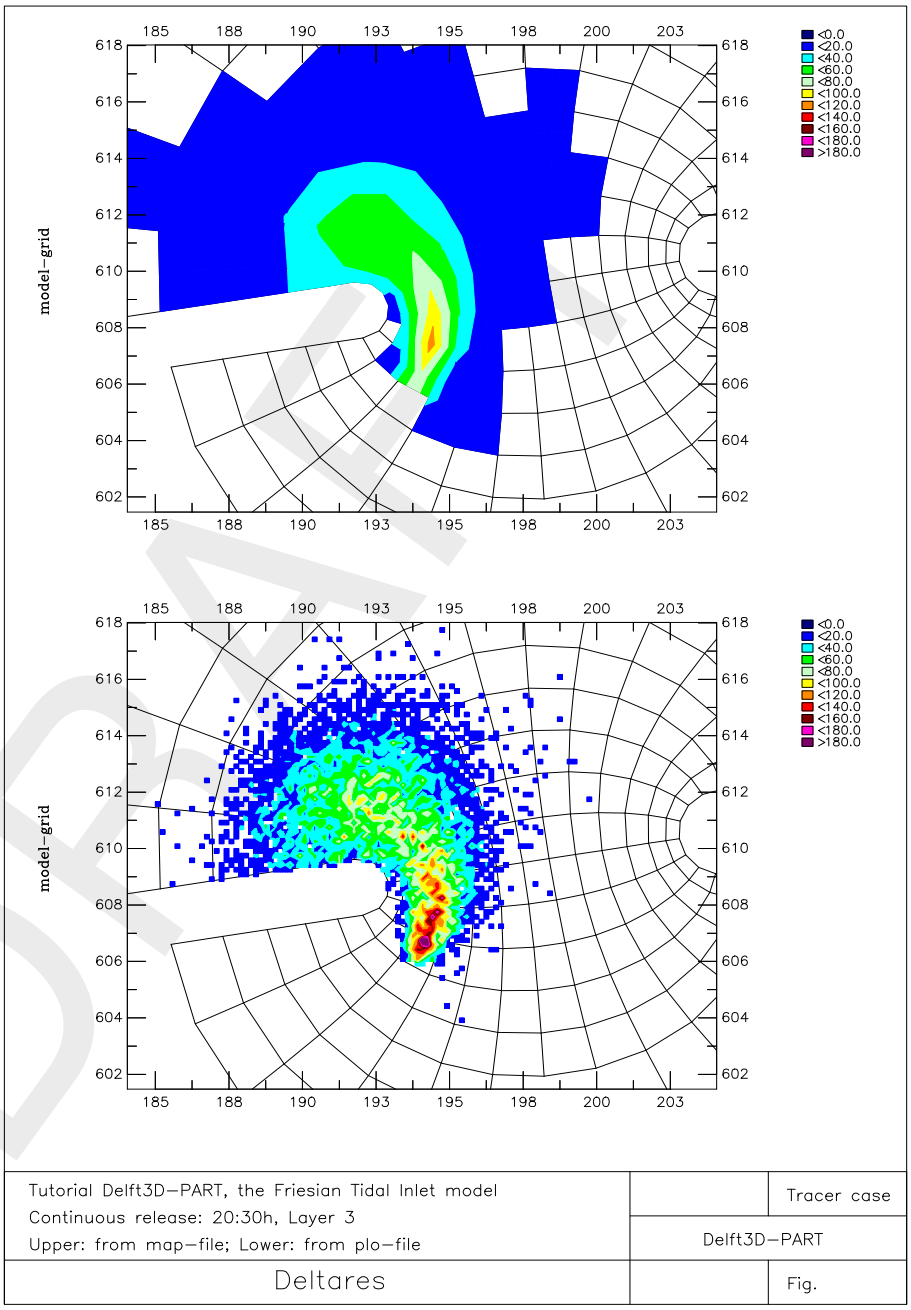

Figure 4.41: *Tracer Case: Continuous release: situation at 20:30 hrs in layer 3: MAP-file (upper) and PLO-file (lower)*

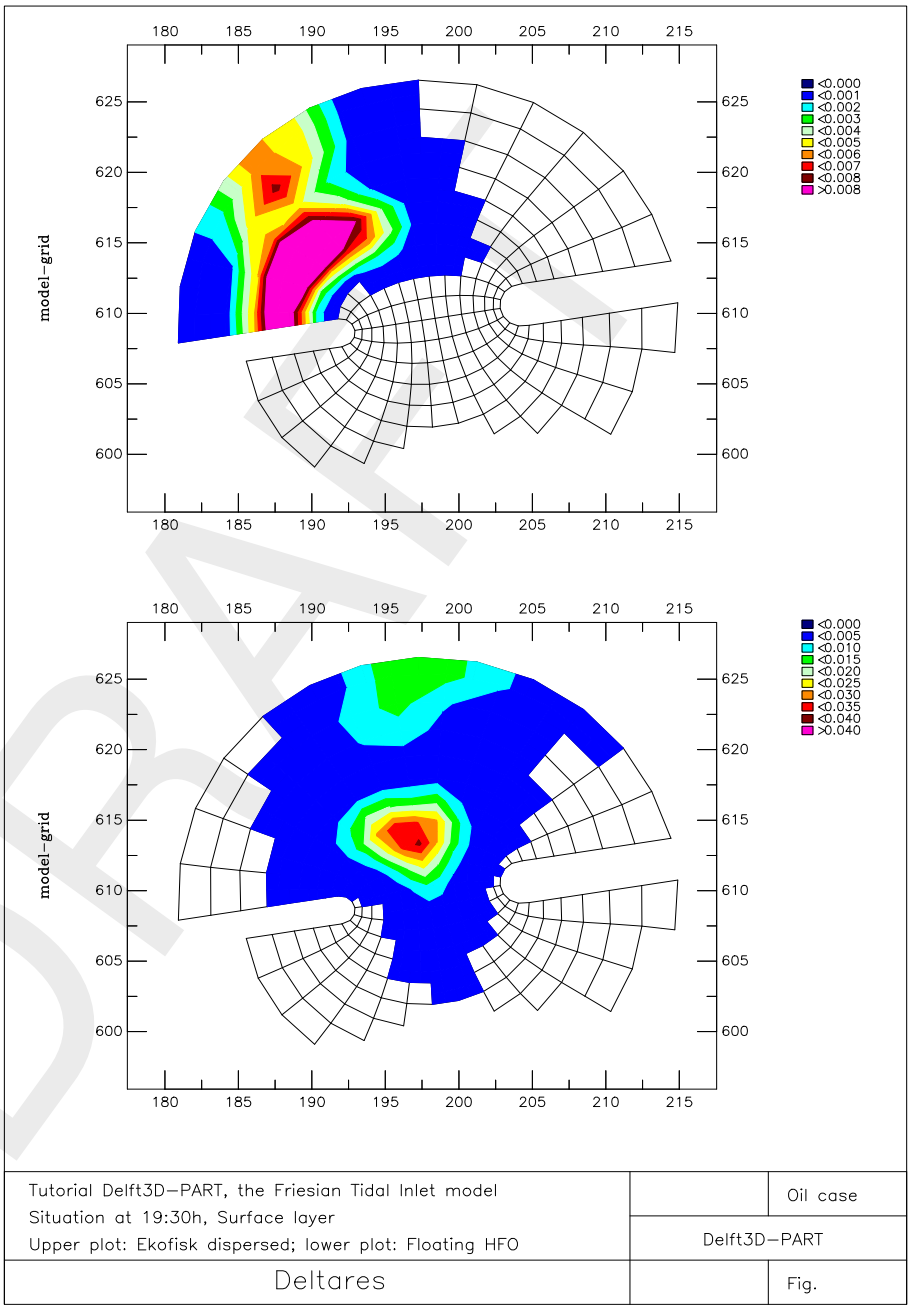

Figure 4.42: *Oil Case: Situation at 19:30 hrs in the surface layer: Ekofisk dispersed (upper) and Floating HFO (lower)*

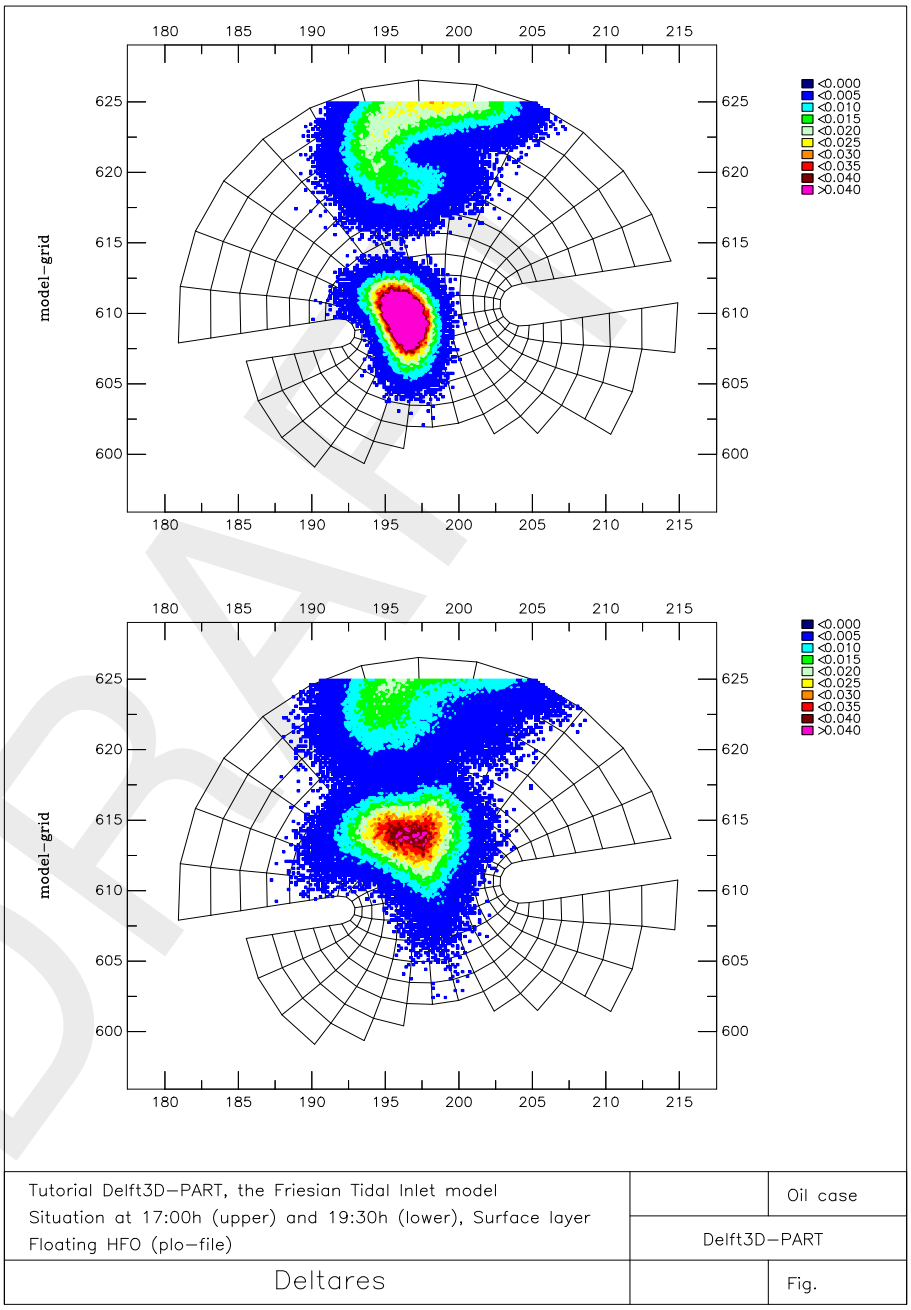

Figure 4.43: *Oil Case: Situation at 17:00 hrs (upper) and 19:30 hrs (lower), PLO-file for Floating HFO in the surface layer*

5 Conceptual model

5.1 Introduction

D-Particle Tracking is a 3-dimensional particle tracking model that is particularly useful for mid-field water quality modelling. It calculates a dynamic concentration distribution by following the tracks of thousands of particles with time. The model provides a detailed description of concentration distributions, resulting from instantaneous or continuous releases of salt, oil, temperature or other conservative or simple decaying substances. This chapter gives you a brief introduction to the computer model and its applications (see also WL | Delft Hydraulics (1993); Van den Boogaard *et al.* (1993)).

5.1.1 Operational functionality

D-Particle Tracking can operate in the following modes:

- Standard mode: 3D or 2DH mode: D-Particle Tracking coupled to 3D or 2DH Delft3D-FLOW or D-Flow FM (one layer model or multi-layer model, sigma-layers and Z-layers (*Note: the combination of sigma- and Z-layers has not been tested*), and extended with an analytical vertical velocity profile for bottom shear and wind.
- Oil spill module: simulation of oil spills with floating and dispersed oil fractions. *(Note: for unstructured grids as used in combination with D-Flow FM the oil model in 3D has not been fully tested yet).*
- Several specialised modes, among which agent-based modelling of fish larvae and other organisms that exhibit independent behaviour. *(Note: not yet implemented for unstructured grids.)*

5.1.2 Physical system

The D-Particle Tracking model is used for water quality modelling. D-Particle Tracking simulates transport processes and simple chemical reactions of substances. The model can simulate detailed shapes of patches of wasted material.

The physical components in the system are:

- The water system: a lake, estuary, harbour or river, possibly with open boundaries to other water systems. Tidal variations are included.
- Outfalls due to human activities.
- Chemical substances like rhodamine dyes, salt, oil or a demand of oxygen due to fast chemical reactions.
- Wind fields.
- Dissolved and/or particulate substances.

5.1.3 Processes

This section describes the D-Particle Tracking model in terms of physical processes or phenomena that the model was designed to represent.

- ◇ The dynamics of patches close to an outfall location.
- ◇ Simple first-order decay processes like the decay of several fractions of oil.
- ◇ Vertical dispersion for well-mixed systems.
- ◇ Horizontal dispersion due to turbulence. According to turbulence theory this dispersion increases in time.
- ◇ The effects of time-varying wind fields on the patches.
- ◇ The effects of bottom-friction on the patches.
- ◇ The existence of a plume at the outfall (rather than a point-source) by starting the simulation from a circular plume with an estimated or field-measured radius.
- ◇ Settling and resuspension of particles.

5.2 Principles of a random walk particle tracking model

D-Particle Tracking is a random walk particle tracking model, which is based on the principle that the movement of dissolved (or particulate) substances in water can be described by a limited (large) number of discrete particles that are subject to advection due to the currents and by horizontal and vertical dispersion. The movement of the particles consists therefore of two elements. For each time-step, the first step is the advection step due to the shear stresses from currents (bottom) and wind (surface). The second step is the random walk step in which the size and direction of the movement is a random process but is related to the horizontal and vertical dispersion. More details are given in chapter 6.

5.3 Dispersion coefficients

5.3.1 Introduction

The dispersion coefficients are the input parameters for the random spreading processes. In the horizontal and vertical direction, the dispersion coefficients are treated separately, even through the numerical treatment is the same.

5.3.2 Horizontal dispersion

The horizontal dispersion coefficient accounts for all of the random fluctuations in the horizontal that are not resolved in the hydrodynamics. For particle tracking simulations, the horizontal dispersion coefficient is also time dependent. In the initial period of time after the release of the particles, the patch of particles is relatively small and the mixing of the particles is caused by small-scale turbulence effects only. However, after some time, the ‘cloud’ of particles will have spread sufficiently such that larger-scale eddies and circulations will now contribute to the mixing effect.

The dispersion coefficient models the effects of *turbulence* that were not included in the hydrodynamics.

Turbulence model

Turbulent diffusion accounts for small scale deviations from the mean hydrodynamic velocity field. These deviations are partially correlated and therefore lead to a net extra displacement. This net extra displacement has a random direction. Therefore it is appropriate to model the effect as dispersion.

Since D-Particle Tracking is a dynamic 3D model dispersion coefficients are small (order 1 m^2/s). The turbulence processes on this scale are time-dependent. We will demonstrate this by using kinetic gas-theory (Csanady, 1973), describing molecular diffusion E:

$$E = \int_0^t \langle \vec{v}(0), \vec{v}(\tau) \rangle \, d\tau \tag{5.1}$$

The bracketed term under the integral is named the Lagrangian correlation coefficient. Using the theory of Brownian motion it can be approximated as:

$$\langle \vec{v}(0), \vec{v}(\tau) \rangle = |v_0|^2 e^{-\tau/t_L} \tag{5.2}$$

with t_L an appropriate time-scale. This expression leads to a diffusion coefficient of the form:

$$E = v_0^2 t_l (1 - \exp(-t/t_l)) \tag{5.3}$$

Note that the two limits of this function are $E = at$ for large t_l and $E = a$ for small t_l. In D-Particle Tracking it is assumed that the dispersion process can be described in the same way and that the dispersion coefficient can be fitted to a function with a power between these two limits ($0 < b < 1$), which leads to:

For the horizontal direction the dispersion coefficient is defined as:

$$D_{x,y} = at^b \tag{5.4}$$

with a and b coefficients that follow from calibrating the model (Bent *et al.*, 1991). The time t is defined from $t = 0$, which is the time at which the given particle, for which dispersion is calculated, is released.

Bed shear stress

The bed shear stress at any location is calculated from:

$$\tau_b = \frac{\rho g (u^2 + v^2)}{C^2} \tag{5.5}$$

with:

τ_b	bed shear stress [Pa]
ρ	water density [kg/m^3]
u	flow velocity in x direction in the bottom layer [m/s]
v	flow velocity in y direction in the bottom layer [m/s]
C	Chézy coefficient [m$^{1/2}$/s]
g	gravitational acceleration [m/s^2]

If the bed shear stress at any location is less than the critical shear stress for sedimentation, a particle that comes into contact with the bottom at that location will remain attached to the

bottom (sedimentation). For sedimentation, D-Particle Tracking creates an extra model layer for sediment at the bed.

If the bed shear stress at any location is greater than the critical shear stress for sedimentation, a particle that comes in contact with the bottom at that location will be reflected back into the water column.

If the bed shear stress at any location is greater than the critical shear stress for erosion, all deposited particles at that location (i.e. particles located in the extra bed-sediment layer) will be returned to the water column instantaneously.

The settling velocity of each particle at time t is calculated from:

$$v_s = c^n \times \left[A_0 + A_1 \sin\left(\frac{2\pi\,(t+\phi)}{T} \right) \right] \tag{5.6}$$

where:

c	local concentration of particles [kg/m^3]
n	exponent for adjusting concentration-dependent settling velocities
A_0	the non-cyclic component of the settling velocity [m/s]
A_1	the amplitude of a periodic sinusoidal variation in time [m/s]
T	the period of the sinusoidal variation [hours]
ϕ	the phase lag for the sinusoidal variation [hours]

The factor in front of the square brackets enables you to define a concentration-dependent settling velocity. If the exponent is set to $n = 0$, the settling velocity is simply a sinusoidal function of time.

Remark:

◇ For negative values of v_s, the particles will move upwards towards the water surface.

5.3.3 Vertical dispersion

In a well-mixed, horizontally uniform flow, the vertical dispersion coefficient may be estimated from the mixing length and the turbulent kinetic energy as:

$$D_z = \frac{c_\mu^{1/4} L \sqrt{k}}{\sigma_C} \tag{5.7}$$

with:

D_z	vertical dispersion coefficient [m^2/s]
c_μ	a constant; ≈ 0.09, calibrated for local equilibrium shear layers (Rodi, 1984)
L	mixing length [m]
k	turbulent kinetic energy
σ_C	Prandtl-Schmidt number ($= 0.7$ for the transport of heat and salinity)

The Bakhmetev (1932) mixing length is estimated by:

$$L = \kappa(H - Z)\sqrt{(Z/H)} \qquad \text{with} \qquad Z = -(z - \zeta) \tag{5.8}$$

with:

κ	von Kármán constant ($= 0.41$)
z	the vertical co-ordinate

ζ	the free surface elevation above the reference plan (at $z = 0$)
d	the depth below the reference plane (bed level $z = d$)
H	the total water depth, given by $H = d + \zeta$

It should be noted that the Z co-ordinate is pointing downwards, i.e. $Z = 0$ is at the surface and $Z = H$ is at the bottom.

The turbulent kinetic energy is assumed to have a linear profile:

$$k = k_b(Z/H) + k_s(1 - Z/H) \tag{5.9}$$

with:

k_b	turbulent kinetic energy near the bottom
k_s	turbulent kinetic energy near the surface

The empirical relationships for the turbulent kinetic energy at the bed and at the surface are taken from the k-L turbulence model used in the hydrodynamic models. This gives:

$$\begin{aligned} k_b &= \frac{u_{*_b}}{\sqrt{c_\mu}} = \frac{\tau_b}{\sqrt{c_\mu}\rho_0} \\ k_s &= \frac{u_{*_s}}{\sqrt{c_\mu}} = \frac{\tau_w}{\sqrt{c_\mu}\rho_0} \end{aligned} \tag{5.10}$$

with:

τ_b	bottom shear stress [Pa]
τ_w	wind stress [Pa]
ρ_0	density of water [kg/m^3]

The shear stresses are derived from the relations :

$$\begin{aligned} \tau_b &= \frac{g\rho_0|v|^2}{C_{2D}^2} \\ \tau_w &= \rho_a C_d |w|^2 \end{aligned} \tag{5.11}$$

with:

g	gravity constant ($= 9.81$ m/s^2)
ρ_a	density of air ($= 1.25$ kg/m^3)
C_{2D}	Chézy coefficient for 2D formulations ($C_{2D} = 50$ m$^{1/2}$/s; unless specified otherwise in the sedimentation/erosion model)
C_d	wind drag coefficient of the free surface
$\|v\|$	advective velocity (computed from Delft3D-FLOW)
$\|w\|$	wind velocity at 10 m above the water surface

The resulting vertical dispersion model (known as the k-L model) is obtained by substituting the above expressions into the expression for the vertical dispersion coefficient to obtain:

$$D_z(z') = \frac{\kappa}{\sigma_C} H(1 - z')\sqrt{z'}\sqrt{u_{*_b}^2 z' + u_{*_s}^2(1 - z')} \tag{5.12}$$

where $z' = Z/H$

Figure 5.1 shows an example of the k-L vertical dispersion coefficient (and its gradient that causes particle drift) for a wind speed of 7.5 m/s.

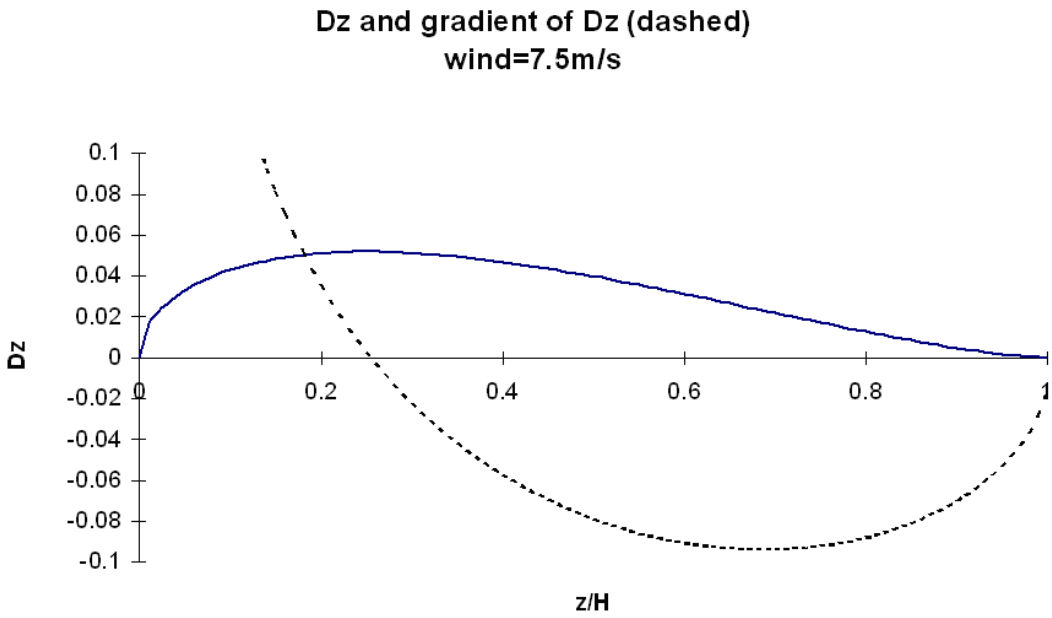

Figure 5.1: *Vertical disperison coefficient [m^2/s] and its gradient (dashed line) as a function of relative depth for the k-L turbulence model, at a wind speed of 7.5 m/s and a Chézy coefficient of 50.0.*

D-Particle Tracking does not use space-dependent dispersion coefficients as this would lead to additional stochastic drift terms. From Figure 5.1, it can be seen that particles would drift towards the bottom and the surface and would accumulate there. In order to prevent such non-physical behaviour, the depth-dependency of the vertical dispersion coefficient is eliminated by depth-averaging. D-Particle Tracking allows linear scaling of the depth-averaged dispersion coefficient to allow for a reduction in vertical mixing due to stratification in the 3D models.

The depth-averaged relation for D_z is obtained by integrating the above expression to obtain:

$$\begin{aligned}\overline{D_z} &= \frac{\kappa H}{\sigma_C}\int_{z'=0}^{z'=1}\sqrt{u_{*_b}^2 z'^2\left(1-z'\right)^2 + u_{*_s}^2 z'\left(1-z'\right)^3}dz' \\ &\approx \frac{\kappa H}{\sigma_C}\left[\int_{z'=0}^{z'=1}\sqrt{u_{*_b}^2 z'^2\left(1-z'\right)^2}dz' + \int_{z'=0}^{z'=1}\sqrt{u_{*_s}^2 z'\left(1-z'\right)^3}dz'\right] \\ &= \frac{\kappa H}{\sigma_C}\left[\frac{u_{*_b}}{6} + \pi\frac{u_{*_s}}{16}\right]\end{aligned} \tag{5.13}$$

5.4 3 Dimensional flow field

D-Particle Tracking is a 3D-model. A 3D hydrodynamic flow field is obtained from a 3D Delft3D-FLOW or D-Flow FM hydrodynamic simulation (operation in mode 1) or by superimposing a logarithmic velocity profile over depth for the bottom shear on a 2DH Delft3D-FLOW (operation in mode 2) simulation and a parabolic profile over depth for wind. In this section the velocity profiles for 2 DH calculations are discussed:

Logarithmic profile for bottom shear

The logarithmic profile for bottom shear is given by:

$$v_z = C \ln\left(\frac{H-Z}{Z_0}+1\right) \times v \tag{5.14}$$

where C is:

$$C = \left[\left(1+\frac{Z_0}{H}\right)\ln\left(\frac{H}{Z_0}+1\right)-1\right]^{-1} \tag{5.15}$$

with:

v_z	vertical profile of the horizontal velocity
Z	depth co-ordinate (from 0 (surface) to H (bottom))
H	water depth
Z_0	roughness length
v	depth-average velocity

The roughness length is of the order 2 cm. The depth-averaged velocity is obtained from a 2DH hydrodynamic calculation.

Parabolic profile for wind

The parabolic profile for wind is given by:

$$v_z = \alpha\left(3\left(1-\frac{Z}{H}\right)-2\right)\left(1-\frac{Z}{H}\right)W \tag{5.16}$$

with:

W	wind speed at 10 m above sea level
α	wind drag coefficient

The wind-drag coefficient is typically in the order of 0.03. The integral over depth is zero and is superimposed on the normal velocity profile which already includes the gross average influence of the wind. This gross wind effect on the velocity field must have been incorporated in the 2DH-hydrodynamic velocity field.

5.5 Oil spill module

The D-Particle Tracking Oil Spill model calculates the transport, spreading, evaporation and dispersion of an oil patch. Transport is either 2D or 3D. Oil can either be floating on the water surface, or it can be transported as a dispersed phase in the water column. Oil dispersion, also referred to as entrainment, is generated by breaking waves (due by wind) according to a formulation of Delvigne *et al.* (1986). Evaporation is based on a simple first order decay process or on formulations by Fingas (FIngas (2004), Fingas (2013)).

Release of oil

Oil can be spilled as an instantaneous release or as a continuous release. The radius of an instantaneous release may follow from the standard input menu of the release, but may also be specified by the following formulation (Fay and Hoult, 1971):

$$R_0 = \frac{k_2^2}{k_1}\left(\frac{V_0^5 g\left(\frac{\rho_w-\rho_0}{\rho_w}\right)}{\nu_w^2}\right)^{1/12} \tag{5.17}$$

with:

V_0	initial volume of the oil spill [m^3]
ρ_0	oil density [kg/m^3]
ρ_w	density of water [kg/m^3]
g	gravity constant
ν_w	kinematic viscosity of water [10^{-6} m^2/s]
k_1, k_2	constants of Fay (1.14 and 1.45)

You should specify the oil density ρ_0 as input. The radius describes a patch after the so-called 'gravity inertial phase' which lasts in the order of 5 minutes for most spills. The thickness of the floating patch is then usually less than 1 mm. It is not recommended to use this description for continuous releases, but to specify the radius of the release according to the information that is available.

Wind induced advection of surface oil

The advection of surface floating oil is subject to wind effects. This is widely published in literature. For example, Labelle and Johnson (1993) carried out simulations of oil-spill trajectories for which each trajectory was constructed using vector addition of the current field and 3.5 percent of the instantaneous wind. A drift angle was computed as a function of wind speed (inversely related to wind speed). In a review by the Task Committee on Modelling of Oil Spills of the Water Resources Engineering Division (1996), it has been reported that the majority of spill models use a simplified linear superposition technique to approximate spill motion. The currents induced by winds and waves are normally lumped together and represented by an empirically based drift factor and deflection angle dependent on the local wind speed and direction. Drift speeds typically vary from 2.5–4.4 % of the wind speed. The deflection angles vary between 0 and 25 degrees to the right/left of the wind direction (northern/southern hemisphere). The most detailed description of drift of oils is given by Yousseff and Spaulding (1993). Here also the drift speed is specified as typically between 2.5 and 4 % of the wind speed with a mean value of 3.5 %, and deflection angles between 0 and 25 degrees, with a mean of 15 degrees. Yousseff and Spaulding (1993) deal in detail with the effects of waves on the transport.

A representation of the effect of wind in D-Particle Tracking is implemented for oil. For a reasonable behaviour of surface floating oil under windy conditions, it is essential for the wind to affect the advection of the surface floating oil. The most important effect is drift as a percentage of the wind speed. The relationship that describes this effect is specified as

$$C_{wd}(V_w - V_f) \tag{5.18}$$

with C_{wd} the wind drag, V_w the wind speed and V_f the current speed. This relationship is only applied to surface floating oil because the dispersed oil will be transported correctly by the currents of the hydrodynamic model and not be directly influenced by wind.

Another factor that affects the transport of the oil is governed by the aforementioned deflection angle, which is an angle between the wind direction and oil advection. This is essentially caused by the fact that the effects of the waves is under the influence of Coriolis and that the wave induced transport is at an angle of the wind. This angle is an empirical parameter. This parameter is chosen to be a constant and it is therefore assumed that the angle does not depend on the wind speed. The deflection angle will depend on the latitude. The deflection angle is included in the D-Particle Tracking model as an additional parameter. The deflection angle would therefore essentially be a calibration parameter, depending on latitude and wind strength.

The drift of the surface oil is implemented in the 3-dimensional mode. When the flow is in a 2D mode, the advection by wind drift at the surface is included in the vertical profile that is derived in D-Particle Tracking (see section 5.4), thus an additional wind drift is not required.

Evaporation of oil

Evaporation of floating oil is implemented as a first order decay process, the rate is either explicitly specified or it is calculated according to the formulations by Fingas (FIngas (2004), Fingas (2013)). Decay can also be specified by a decay constant as usual in the menu of process parameters (this can be done with a time-series), or by defining a fixed fraction of oil that decays each day.

Fingas proposed to describe the time-dependent evaporation using a natural log or a square root function, with a temperature dependency (F. (2011)):

For oils (most oils and petroleum products) that follow a logarithmic equation:

$$\text{Percentage evaporated} = [.165(\%D) + .045(T - 15)]\ln(t) \tag{5.19}$$

For oils like diesel fuel that follow a square root equation:

$$\text{Percentage evaporated} = [.0254(\%D) + .01(T - 15)]\sqrt{t} \tag{5.20}$$

where:
$\%D$ is the percentage (by weight) that evaporates at 180^oC
T the water temperature in ^oC
t the age (time sicne release into the water) in minutes.

Within the D-Particle Tracking model the formulation with the logarithm or the square root is selected via the water temperature: A positive temperature is used to select the logarithm and a negative temperature to select the square root formula.

Thus, with the evaporation description these two parameters will need to be supplied by the user:

- the (water) temperature
- the mass percentage oil evaporated at 180^oC

It is known that oil contains fractions that do not evaporate. For example, Reed (1989) adopted in his model a mass transfer coefficient that uses the molecular weight of the volatile fraction of the oil spill.

In the oil module of PART, a volatile fraction has been introduced, albeit simplified compared with the implementation of Reed (1989). It is assumed that the volatile fraction F_{vol} evaporates as a first order process (i.e. exponential), and that the non-volatile fraction does not evaporate at all. This is achieved by the introduction of the following:

$$\frac{dF_v}{dt} = -\left(\frac{F_{vol} - F_v}{1 - F_v}\right)k \tag{5.21}$$

Where F_v is the evaporated fraction and k the evaporation rate constant. The numerator in the equation should always be positive and if $F_{vol} - F_v < 0$ then the evaporation is set to zero.

The oil viscosity will change during the evaporation process. In the literature, descriptions of the dependency of the viscosity as a function of the evaporated fraction exist and is generally given as:

$$\eta = \eta_0 e^{(C_v F_v)} \tag{5.22}$$

This equation is given for the dynamic viscosity. Assuming that the density is approximately constant throughout the simulation, then the same function can be used to describe the kinematic viscosity. Reed (1989) states that the value of C_v in his model is equal to 1 for gasoline, kerosene and light diesel fuel and 10 for other petroleum products. In the D-Particle Tracking model, this is implemented by assuming that $C = 1$ is used for light oils (kinematic viscosity less than 500 cSt) and $C = 10$ for the heavy oils (viscosity greater than 500 cSt).

Dispersion (entrainment) of oil

Dispersion of floating oil, or entrainment of oil in water, is implemented as a zero order decay process, i.e. the entrainment rate is independent of the floating oil concentration. The dispersion rate of oil depends only on the wave energy that is dissipated by the patch, and the type of oil.

The dispersion rate can be calculated in three ways:

- As a constant fraction per day (so independent of wind and waves).
- According to the formulation by Delvigne and Sweeney, as shown below, where the threshold for the wind velocity where white capping occurs is 5 m/s.
- According to the formulation by Delvigne and Sweeney, but with a wind velocity threshold that is user-defined.

In the second and third option, the dispersion rate Q [kg/(m^2/s)] of oil is given (see Delvigne and Sweeney (1988); NOAA (1994); Delvigne and Hulsen (1994)) by:

$$\begin{aligned}
Q &= \int_{delta_{\min}}^{\delta_{\max}} Q(\delta)\ \mathrm{d}\delta \\
Q(\delta) &= C'' D_e^{0.57} F_{wc} N(\delta) \delta^3 \\
N(\delta) &= N_0 \delta^{-2.3} \\
D_e &= 0.0034 \rho_w g H_0 / \sqrt{2} \\
H_0 &= \frac{0.243 U_w^2}{g} \\
F_{wc} &= \frac{f_w}{t_p} \\
t_p &= 8.13 \frac{U_w}{g} \\
f_w &= \max(0, 0.032(U_w - 5.0))
\end{aligned} \tag{5.23}$$

with:

Q	dispersion rate [kg/(m^2/s)]
$Q(\delta)$	dispersion rate per unit of diameter for droplets of diameter d [kg/(m^2/s)]
δ	oil droplet diameter [m]
$\delta_{\min}$	minimum oil droplet diameter [m]
$delta_{\max}$	maximum oil droplet diameter [m]

C''	oil constant (calibration parameter, depending on kind of oil)
$N(\delta)$	oil particle size distribution function
N_0	normalisation constant distribution function
D_e	dissipation of wave energy per unit surface area [J/m^2]
F_{wc}	number of waves that break per wave period [-]
t_p	peak wave period [s]
U_w	wind speed [m/s]
f_w	fraction of sea covered by white caps [-]

Here, white capping is formulated according to Holthuijsen and Herbers (1986) with the initial wind speed for white capping equal to 5 m/s. The minimum droplet size $\delta_{\min}$ can be taken zero as a good approximation. The crux is knowledge of parameters $\delta_{\max}$, N_0 and the calibration constant C''.

According to NOAA (1994), after resurfacing of particles back into the oil slick, $\delta_{\max}$ can be taken equal to 70 μm. In this approximation, it is assumed that after each breaking wave a quasi-steady state distribution of droplets results, i.e. the resurfacing of particles back into the oil slick due to buoyancy goes fast compared with the dissipation of wave energy by the oil slick. Defining a new calibration constant C_0 the following expression results for Q:

$$Q = 5.08 \cdot 10^{-8} C_0 S_{\text{cov}} D_e^{0.57} F_{wc} \tag{5.24}$$

with

Q	dispersion rate [kg/(m^2/s)]
C_0	oil constant (calibration parameter)
S_{cov}	proportion of the sea surface covered by the oil in the relevant area
D_e	dissipation of wave energy per unit surface area [J/m^2]
F_{wc}	number of waves that break per wave period [-]

The calibration parameter C_0 depends on the kind of oil: oil with a high viscosity disperses hardly for a wind speed of 10 m/s whereas oil with a low viscosity disperses fast for such a wind speed.

An order of magnitude of C_0 follows from Delvigne and Hulsen (1994) (Table 2 and Figure 4 of that publication). Since Delvigne and Hulsen do not take into account a steady state assumption their values can only be a first estimate for D-Particle Tracking. Estimates of the dispersion constant C_0 are:

$C_0 \approx 2000$ for Ekofisk with standard oil viscosity $\nu = 8$ cSt (at 20 °C)
$C_0 \approx 50$ for Heavy Fuel Oil with standard oil viscosity $\nu = 3000$ cSt (at 20 °C)

Since viscosity is temperature dependent C_0 depends both on oil type and on temperature. Temperature dependence may be neglected for low viscous oils with $\nu < 100$ cSt (Delvigne and Hulsen, 1994).

Delvigne and Hulsen (1994) have shown that there is a relationship between the C_0 and the oil viscosity. Since viscosity is an oil characteristic and used as input of the model, this relationship is included in the model. The relationship used in the modified PART(Oil) model is based on the data published by Delvigne and Hulsen (1994). The data was examined and a log-log plot revealed that this relationship can be specified by two equations (Figure 5.2). The equations used and the goodness of fit with the data are indicated in the figure.

In order to calculate the entrainment flux, some representation of surface area for each surface oil particle is required. In the oil module an area for each particle is derived, based on the mass

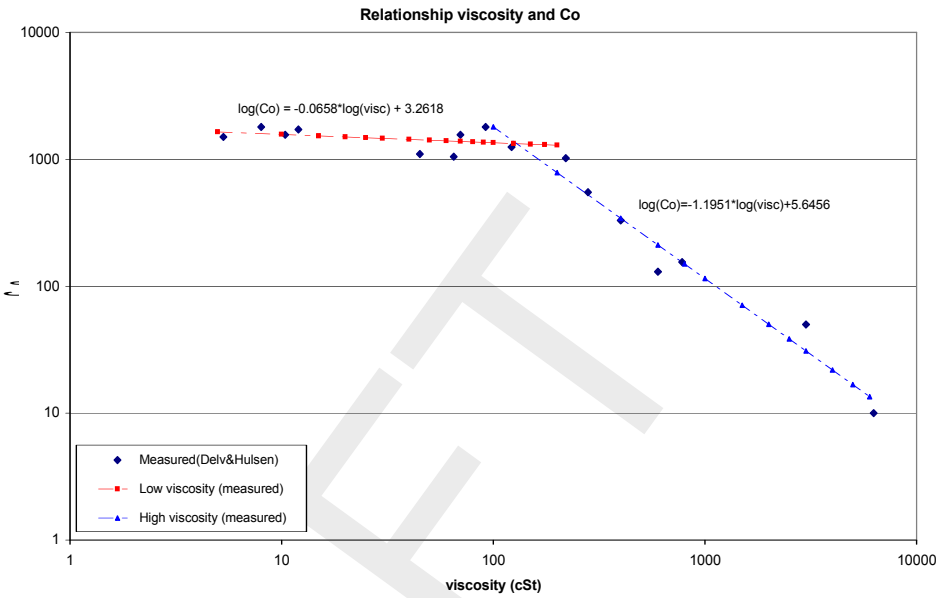

Figure 5.2: *Relationship between viscosity and the dispersion parameter C_0 (Delvigne and Hulsen, 1994)*

of surface oil associated with this particle (WL | Delft Hydraulics, 2003). This is calculated using an assumed oil layer thickness. Validation with the oil budget model ADIOS has resulted in an optimal value of 0.00005 m. This value of 0.05 mm (50 μm) is also similar to the value of 70 μm generally used to define the oil droplets that remain in suspension.

Emulsification

Water-in-oil (w/o) emulsions form a viscous cream, or floating, coherent semi-solid lumps, often called *chocolate mousse*. The process depends on oil composition. The formation of w/o emulsions reaches a maximum between 10 and 100 hours (Wheeler, 1978). The emulsification process itself is relatively rapid. It has been reported that emulsification takes place fully in the laboratory in 0.1–3 hours (Fingas *et al.*, 1999).

Emulsification is virtually an irreversible process (Wheeler, 1978) and changes the liquid to a heavy, semi-solid material (Fingas and Fieldhouse, 1996) with a high viscosity. Viscosity can be as high as $4 \cdot 10^6$ cP (Bos, 1980).

The emulsification process is implemented in D-Particle Tracking following the algorithm presented by Mackay and others (Mackay *et al.*, 1980; Zagorski and Mackay, 1982), in which the rate of water uptake $\tilde{F}_{wc}$ is given by:

$$\tilde{F}_{wc} = C_1 \left(U_w + 1\right)^2 \left(1 - \frac{F_{wc}}{C_2}\right) \tag{5.25}$$

with U_w the wind speed, F_{wc} the water content and C_1 and C_2 model parameters. C_1 is given as $2 \cdot 10^{-6}$ for emulsifying oils and 0 for others, whilst C_2 is a constant controlling the maximum water content and is suggested to be 0.25 for home heating oil and 0.7 for crude and heavy fuel oil (Reed, 1989). In several other publications, however, the maximum water content for these heavy oils is said to reach values of 75–80 % (for example, Huang (1983)). The switch of C_2 between 0.25 and 0.75 is made at a viscosity of 500 cSt, whilst the value of C_1 (0 or $2 \cdot 10^{-6}$) is selected by the user and thus dependent on the emulsion formation tendency of the oil in question.

The main effect of emulsification (increase in the water content) in the model is the change in viscosity and is given as:

$$\frac{\mu}{\mu_0} = e^{\left(\frac{2.5F_{wc}}{1.0-C_3F_{wc}}\right)} \tag{5.26}$$

As with the change of viscosity as a function of the evaporated fraction, it is assumed that the density does not change significantly, compared with the changes in viscosity and is assumed constant. Thus the implementation in the PART(Oil) model uses the kinematic viscosity in the aforementioned equation instead of the dynamic viscosity. The constant C_3 is suggested to be 0.65 (Reed, 1989).

Emulsification does not only affect viscosity (and therefore the dispersion (entrainment) process) but also evaporation. According to Fingas (1994), the effect of emulsification is that the viscosity rises two to three orders-of-magnitude, the spreading rate decreases by a similar value and evaporation nearly ceases.

In order to achieve a link between the emulsification and evaporation in PART(Oil), the water content of the emulsion is used to reduce the evaporation rate. In the implementation in PART, it is assumed that the evaporation ceases when the water content has reached its maximum. This maximum water content is oil type dependent. The evaporation rate is adapted when emulsification occurs by reducing the volatile fraction. This is implemented as follows:

$$F_{ew} = \frac{C_2 - F_{wc}}{C_2} F_{vol} \tag{5.27}$$

Where F_{vol} is the volatile fraction of the spilled oil and Few the adapted volatile fraction, replacing the volatile fraction F_{vol} in Equation (5.21). Thus, when the water content reaches its maximum C_2, the adapted volatile fraction reduces to zero and the evaporation halts.

The onset of emulsification can be delayed until evaporation causes the oil characteristics to reach the criteria for emulsification. This delay has been implemented in PART(Oil) by introducing a fraction evaporated oil at which emulsification is initiated (E_v).

Oil density

The density of the oil is affected by evaporation and emulsification. Density is also a function of temperature. In PART, the ADIOS formulation is used, without the dependency of the evaporated fraction and temperature. Hence, in PART, the density can only change when the oil emulsifies. The density is then a linear interpolation of the densities of water and oil, according to their relative content:

$$\rho_{em} = F_w \rho_w + (1 - F_w)\, \rho_{oil} \tag{5.28}$$

where

ρ_{em}	Density emulsion [kg/m^3]
F_w	Water fraction
ρ_w	Water density [kg/m^3]
ρ_{oil}	Oil density [kg/m^3]

Sticking of oil

Oil may stick to land and cause damage to ecological sites. In order to simulate the process of oil sticking to land or to the bed of the water column, a sticking probability must be specified. A particle may come into contact with land due to wind effects or horizontal dispersion and it may come into contact with the bed due to vertical dispersion or settling. The particle sticks to the land or bed if a randomly chosen number between 0 and 1 is smaller than the sticking probability given.

Settling of oil particles

Dispersed oil may settle. However, this velocity is generally negative since oil particles are lighter than water. Most oil and refined products are less dense than water, which means they will float when initially spilled. Experience has shown that oil slicks that initially float will remain buoyant even after weathering. The two circumstances under which oil has been noted to sink occur when the oil is mixed with mineral sediment in the water column or when it is burned in-situ, creating a residue that may be of high density.

Weathering of oil

In addition to the processes mentioned earlier, other weathering processes may affect the presence of oil. Processes such as oxidation, bacteriological decay can in D-Particle Tracking be simulated by means of a first order decay, for which a decay parameter can be specified.

5.6 Data requirements for the conceptual model

A list of data that enter the conceptual model and pertain to the physical system that is being modelled will be described in this section. Assumptions are made about the sensitivity of the model results for these parameters. These assumptions are general remarks and their importance strongly depends on the accuracy required by you for giving you enough insight in the particular water quality problem at hand.

1 *Hydrodynamic database of volumes and flows*

Source	supplied by the coupling module in Delft3D-FLOW or D-Flow FM
Meaning	determines the advective transport and the amount of water available for dilution of the wasted substance
Sensitivity	should be accurate, especially for the calibration of dye experiments

2 *Wind drag coefficient*

Source	user-defined
Meaning	parabolic wind profile over depth (2D flow field); drag on surface oil (Oil module).
Sensitivity	anisotropy of a patch for a dye experiment depends on this parameter (range 1 %–5 %). Experience at Delft Hydraulics learns that a value of 1 % is mostly used for D-Particle Tracking applications rather than the 3 % recommended by literature. This may be due to the D-Particle Tracking algorithm (parabolic profile and depth-averaged vertical dispersion coefficient).

3 *Wind field*

Source	user-defined
Meaning	describes parabolic wind profile for 2D FLOW velocity field, used in the 2DH approach. If the depth-averaged vertical dispersion option is selected, then the wind is also used to calculate the ver-

	tical dispersion. For the oil module, the wind is used to calculate the entrainment flux of the oil into water.
Sensitivity	the average direction and wind speed should be a reasonable estimate

4 *Deflection angle (3D)*

Source	user-defined (literature value), depending on latitude
Meaning	describes the angle between the wind direction and oil advection.
Sensitivity	The deflection angle is generally between 0 and 25 °rotating to the right on the northern hemisphere and to the left on the southern hemisphere.

5 *Roughness length (2DH model)*

Source	user-defined (literature value)
Meaning	describes logarithmic profile due to bottom shear for 3D velocity field
Sensitivity	a value of 2 cm is recommended

6 *Dispersion parameters a and b for horizontal dispersion*

Source	user-defined
Meaning	determines the increase of the horizontal dispersion coefficient with time.
Sensitivity	the parameter a is most important for the short-time range whereas b is most important for the long-time range. The value of the parameters depends on the amount of detail (turbulence) not incorporated in the hydrodynamics. The parameters should follow from calibration or from an expert opinion.

7 *Amount of released material*

Source	user-defined
Meaning	an instantaneous release (mass) or a continuous release (release rates and concentrations or, alternatively, mass rates).
Sensitivity	quantitative results depend linearly on the accuracy of these input data

8 *Time and location of released material*

Source	user-defined
Meaning	-
Sensitivity	should be accurately known

9 *Constants oil spill module*

Source	user-defined, including oil-viscosity, from which the dispersion (entrainment) parameter is derived, see Delvigne and Hulsen (1994). A stickyness probability is important for sticking of oil to land or the bed. All oil model parameters are related to the oil characteristics. Oil characteristics are available from oil databases.

6 Algorithmic implementation

6.1 Introduction

For each particle, transport is split in a part for advection and a part for wind and horizontal and vertical dispersion. Dispersion and advection of clouds of particles are treated with different numerical schemes. These schemes are described in this section.

6.2 Advection schemes

The advective part is solved with an analytical integration procedure that integrates exactly a linearly interpolated hydrodynamic velocity field. The advective velocity of a particle is obtained by linear interpolation of the velocities at the borders of the computational cells of the grid of the hydrodynamic simulation. A vertical velocity profile is added to the interpolated velocity field. The path of a particle in a computational grid-cell is determined by analytical integration along the velocity field. This procedure leads to mass-conservation of water. The analytical integration method automatically deals with closed (land) boundaries correctly, since velocities vanish asymptotically at the borders. Particles that pass open (water) boundaries are taken out of the calculation.

The analytical integration procedure is given by:

$$x(t+\Delta t) = x(t) + \int_0^{\Delta t} \left(\frac{dx}{dt}\right) dt \tag{6.1}$$

with:

x	is the distance
t	is the time
$\frac{dx}{dt}$	is the velocity in x-direction

$$\begin{aligned} x &= x(s(t)) \\ \frac{dx}{dt} &= \frac{ds}{dt}\left(\alpha_x x(s) + \beta_x\right) \\ \alpha_x &= C(\sigma)\left(\frac{Q_+ - Q_-}{V}\right) \\ \beta_x &= C(\sigma)\frac{Q_{+/-}}{V} \end{aligned} \tag{6.2}$$

with:

$s(t)$	is the streamline distance function
$\alpha x(s) + \beta$	the linearly interpolated velocity in the grid along the stream line
$Q_{+/-}$	is the flow though the upwind or downwind surface of the grid cell
V	is the volume of the grid cell
$C(\sigma)$	is the distance between the velocity points in the hydrodynamic grid
$\frac{Q_{+/-}}{V}$	is 1/travel time of the grid cell with this $Q_{+/-}$

For the implemented numerical integration, the path acceleration is neglected:

$$\frac{ds}{dt} = 1 \tag{6.3}$$

This flow field is exactly related to the hydrodynamic flow field (Delft3D-FLOW or D-Flow FM).

The flow field is volume-conserving if:

$$\frac{\partial}{\partial x}\left(\alpha_x x + \beta_x\right) = 0 \tag{6.4}$$

and for coupling to Delft3D-FLOW this condition is satisfied.

6.2.1 Difference between structured and unstructured grids - Delft3D-FLOW and D-Flow FM

The above overview does not make a distinction between the underlying algorithms for the two types of grids. This section is meant to provide some insight:

- ◇ Structured grids, in which all grid cells have a quadrangular shape, allow for a straightforward approach. Here the particles are traced within the grid cell until they leave the cell and then the trajectory in the new cell is calculated. This continues until the particles have been fully traced over the entire time step.
- ◇ The unstructured grids that are used by D-Flow FM, allow for combinations of triangles and quadrangles and even other polygons. The tracing of the particles is done by first splitting up the grid cells into constituent triangles and then constructing the trajectories within these triangles. This means that the flow field as known from the hydrodynamic model has to be split up in a consistent (volume-conserving) way per triangle. Then the trajectories can be calculated in much the same way as for structured grids. The main difference therefore lies in the treatment of the grid cells and the flow field, not in the transport of the particles.

Because of the need to implement a new algorithm (though based on the same philosophy) not all features of the "structured" mode have yet been implemented for the "unstructured" mode as well.

6.3 Dispersion schemes

The dispersive part is solved with an Euler-type numerical scheme. In the horizontal direction also additional advection due to wind (in 2DH mode) is handled with this numerical scheme. In vertical direction a displacement due to settling can be added to the vertical displacement due to dispersion. Boundary conditions are handled simultaneously for these two schemes and are purely reflective.

Dispersion in both the horizontal and the vertical direction is based on a white noise process with a uniform probability density function with zero mean ranging between -1 and +1. The maximum displacement of each particle for each time-step is then:

$$\Delta S = \sqrt{6D\Delta t} \tag{6.5}$$

It is noted here that the dispersion is assumed to be more or less isotropic, so no preferential direction.

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A Input files D-Particle Tracking

A.1 Introduction

The particle model gets its information from the hydrodynamic model (Delft3D-FLOW) and a user input file. An input file is normally generated by the Graphical User Interface (GUI) but may also be edited directly using any text editor. However, you should always be careful when editing the input file directly, since inconsistencies in the input that would not be possible when using the GUI, may lead to unexpected results, without generating appropriate error messages.

This appendix describes the main ASCII input file for D-Particle Tracking. In addition to this input file, PART also requires the file <*runid*.mdp> (see **??**) and the hydrodynamics files generated by the coupling program.

If the oil module is selected and initial condition is specified, an external initial condition file <∗.ini> will be required. The format of this file is in Section A.6.

A.2 General set-up of the input file

Formats

The user input file is free formatted. You may insert information anywhere on lines and may insert comment lines or comments on data lines in the following way:

- ◇ All information after a semicolon (;) is treated as comment, the semicolon included. (This holds also for semicolons in character fields!)
- ◇ Blank lines are skipped and may be used freely.
- ◇ Character strings must be supplied in quotes.

The FORTRAN language may (sometimes) have problems with two subsequent leading zeros in a number, so it is advised not to use multiple leading zeros in the free formatted input.

Errors in input

The input program checks as much as possible for wrong input. It is advised to review the input and run report file carefully. Error messages are not given on screen but only given in the report file, so always check the report file!

Specification of time functions

Time-functions are always specified by a number of breakpoints (days, hours, min, sec), followed by a value for that breakpoint. The program requires the first breakpoint of the time-series to be the same as the start of the simulation and the last breakpoint to be the same as the end of the simulation.

By default, the program carries out a linear interpolation between the break points for all specified time-functions. The program can mimic block functions by specifying two subsequent records with equal time and distinct values. For continuous releases you can select a block function or linear interpolation of the time-function.

Information in the input file

In this section the input file for model type 2 — oil simulation — is defined (2.5 DH or 3D modes). In the explanation of the input file the following symbols are used:

- this item must be specified on a new line.
- $*$ this item must be specified in the input line on the same line as the last line starting with a '-').
- Δ indicates that this input is optional, or its use is only required when some other variable indicates this (since it is > 0).

ASCII Input file (definition of):

```
'V3.66.00        '  ; please, don't change this line

'Tutorial \DPART'
'Friesian Tidal Inlet model'
'Ekofisk and HFO release'
'T0: 1990.08.05 00:00:00 (scu =       ls)'
```

- Run identification.
  The run identification consists of 5 strings of at most 40 characters. The first line is required and identifies the PART version number that is used. This line should not be changed since the model will not run when the version number in the input file is not consistent with that of the model. The subsequent 4 lines are for information purposes and are used on the graphical output. Do not put any quotes in the strings since this will lead to blocking errors that are difficult to trace back.

```
;                          Hydrodynamics file (*.hyd)
'com-tut_fti_part.hyd'; name of *hyd file
;
```

- Name of Delft3D <∗.hyd> file (see **??**).
  This filename consists of at most 80 characters. The file needs to be located in the working directory. The file is generated by the coupling program and contains all the input and output filenames, including the ASCII input file discussed here. It should be noted that the information in the <∗.hyd> file is used by the PART-GUI. When the GUI is exited the <filename.dat> file is generated. This file includes the filenames and locations of the hydrodynamics that will be used. Thus when executing D-Particle Tracking, the information from the <filename.dat> file is used, and not the <∗.hyd> file.

```
;                              Numerical parameters
; Type of model: 1 - tracer (basic module)
;                2 - (obsolete option)
;                3 - (obsolete option)
;                4 - oil model
;                5 - (obsolete option)
  4   0    0    0  ; type of model  tracks(0/1)  extra_output(0/1)  sed/erosion(0/1)
```

- An integer specifying the model-type (or 'mode') — see **??**.
  - $*$ An integer specifying whether particle tracks for all particles are generated in the output. A value of 0 indicates no particle tracks output. A value of 1 will generate output for each calculation time step. A value higher than 1 will be used as a multiplier for the time step at which the tracks are written (this option is not supported by the user interface). It is recommended to keep the number of particles in the model small (e.g. less than 1 000) or use a high multiplier, because the output file can become very large if a large number of particles is used. When the number of particles is greater than 1 000, a warning is generated.
  - $*$ An integer that is no longer used, but is required in the input file.
  - $*$ An integer specifying whether sedimentation/erosion processes are switched on (1) or off (0).

```
        1     900       ; num. scheme            time step(s)  (0=flow time step)
```

- An integer indicating the numerical scheme for advection of the particles (option 1 is the only option available).
  - ∗ An integer indicating the time-step in seconds. A value of ‘0’ means that the time-step will be the same as that of the hydrodynamic database.

```
      1   0.10    0       ; vert. disp option(*)   scale          disp_coeff.(m2/s)
                          ; (*) 0=constant 1=depth averaged
```

- An integer indicating the numerical scheme for vertical dispersion of the particles.
  For the recommended option 0, a constant vertical dispersion parameter is used. For option 1 this parameter follows from an algebraic $k - L$ model.
  - ∗ A real indicating a scale factor for vertical dispersion.
  - ∗ A real indicating a vertical dispersion constant when dispersion option ‘0’ was used. When option ‘1’ is used this value is not used.

```
;                                 Substances
       6       2   ; no of substances         no of oil fractions
 'Ekofisk        '
 'Ekofisk        disp'
 'Ekofisk        stick'
 'Heavy Fuel Oil'
 'Heavy Fuel Oil disp'
 'Heavy Fuel Oil stick'
```

- An integer specifying the total number of substances.
  - ∗ An integer specifying the number of oil substances
- Substance name.
  For each substance, a string of 20 characters (maximum) must be given. For the oil spill module, for each oil fraction, specify 3 names in the following order:
  1. Name of the floating Oil, e.g. ‘Ekofisk’;
  2. Name of the dispersed Oil, e.g. ‘Ekofisk dispersed’;
  3. Name of the Sticking Oil, e.g. ‘Ekofisk sticking’.

  Because of this, we advise to use a substance name with a maximum of 10 characters each, so that the sub-types dispersed and sticking can be added.

```
;                                 Particles
    20000 ;number of particles
```

- Number of particles.
  You may select the total number of particles to be used. More particles results in a more accurate solution of the mathematical equations (not necessarily in a better simulation) and a better resolution of the concentration, but in a longer computation time. The maximum number of particles is limited by the memory of your computer.
  Please note that this number is not necessarily the total number of particles used in the simulation. This is because the total number of particles in the simulation will be the sum of all percentages of particles that is specified for every release (continuous and instantaneous) multiplied by the specified number of particles. Thus the number entered here represents a total release of 100 % of the particles (see instantaneous and continuous releases).

```
;                                 Physical parameters
           0.002 ; roughness [m]
            0.07 ; a coeff. in hor. diff. D = a*t^b
             0.7 ; b coeff. in hor. diff. D = a*t^b
               3 ; wind_drag (%)
            1024 ; density of water (kg/m3)
```

- Roughness length [m].
  The roughness length parameter is one of the calibration constants (see the report concerning the principles of the model). It is advised to take something like 0.02 m. This constant is only used when D-Particle Tracking runs in 2DH mode, but must also be supplied for 3D calculations.
- Isotropic dispersion coefficients [m^2/s].
  This constant a is also subject to calibration. See section 5.3 for details.
- Exponent for horizontal dispersion coefficients.
  This constant b is also subject to calibration. See section 5.3 for details.
- Wind drag coefficient [%].
  This constant represents the velocity of the top most water layer as a percentage of the wind velocity (e.g. 3.0 means 3 %). For the tracer module, this constant is only used when D-Particle Tracking runs in 2DH mode, even though it must also be supplied for 3D calculations. The value is also used by the oil module for the transport of the surface floating oil (2DH and 3D mode).
- Density of water [kg/m^3].

```
 ;                                Wind parameters
  2
; dd hh mm ss        speed(m/s)   direction(degr.)

   0 12 30  0           6.000     270.000
   0 20 30  0           6.000     270.000
```

- the number of “breakpoints” for the time function as an integer.
  That number of records consisting of:
  - 4 integers giving the time of a function point (day, hour, minute, second), followed by 2 reals indicating the wind speed [m/s] and the direction (degrees from the North, e.g. 270 degrees is from the West).

  At least two breakpoints should be given (also for zero wind velocities). The start time and end time of the series of breakpoints (which must be a series increasing in time) should be equal to the start time and stop time of the total simulation.

```
 ;                                Model specific parameters

 ;                                Oil model parameters
    0 ;number of constants
```

- model specific constants (real).
  For the tracer model, there are no additional constants and 0 should be entered. For the oil module additional constants are required.

△ That many records specifying the values of the constants (only required for the oil module, see section 5.3.

```
 ;                                Timers
 ;yyyy mm dd hh mm ss
           0 12 30  0      ;simulation start time
           0 20 30  0      ;simulation stop time
           0  0  0  0      ;DELWAQ take over time
           0 12 30  0      ;map file start time
           0 20 30  0      ;map file stop time
           0  1  0  0      ;map file time step
           0 12 30  0      ;his file start time
           0 20 30  0      ;his file stop time
           0  1  0  0      ;his file time step
  1990  1  1  0  0  0      ;reference date for output
```

- Simulation timers (days, hours, min, sec).
  Two sets of 4 integers, expressing the day, hour, minute and second of the start and the stop of the simulation. The start time must be the same as the start time of the coupled hydrodynamic output file. This is tested by the system. The end time may exceed the end

time of the coupled hydrodynamic simulation. In that case, the hydrodynamics database is rewinded automatically and re-used.

- D-Water Quality delay time (days, hours, min, sec).
  One set of 4 integers defining day, hour, minute and second. This option is no longer supported in the GUI and it is required to set the 4 integers to 0, otherwise unexpected results may occur.
- Map file timers (days, hours, min, sec).
  The map file is used for movie generation (as with the D-Water Quality map file). Three sets of 4 integers must be provided, giving the day, hour, minute and second of the start of the map file, the stop of the map file and the time step in the map file. This output generates concentration distributions mapped on the hydrodynamic grid (optionally aggregated in the vertical).
- Time history file timers (days, hours, min, sec).
  The time history file is used for time histories that can be plotted with GPP. Three sets of 4 integers must be provided, giving the day, hour, minute and second of the start of the file, the stop of the file and the time step in the history file. In this file a time-series of concentrations is given at specified observation points ('monitoring stations'), specified below.
- Time offset (year, month, day, hour, min, sec).
  To map the model time to real world timings, 6 integers must be provided for the year, month, day, hour, minute and second to be added to the model time to obtain the real world time.

```
 ;                                Observation points
    1
;                                      x-coordinate           y-coordinate
   'waste point'                           13210.00               14000.00
```

- An integer giving the number of observation points, also called 'monitoring stations'.
  The observation points are used to generate time histories that can be plotted in GPP (see also the block 'timers' discussed above).

Δ For each observation point supply one line with three items, namely:

- a string of at most 20 characters giving the name of the observation point.

$*$ the x-co-ordinate and y-co-ordinate of the observation point. The co-ordinates must be consistent with the co-ordinate system of the hydrodynamic simulation.
  NOTE: the z-co-ordinate of observation points need not be supplied since in 3D simulations always concentrations for all layers will be given in the history file.

```
 ;                                Output parameters
 ;Zoom grid output method
 8
; dd hh mm ss        recovery(-) (for scaling of output)
   0 12 30  0           1.000
   0 12 45  0           1.000
   0 13  0  0           1.000
   0 14  0  0           1.000
   0 16  0  0           1.000
   0 18  0  0           1.000
   0 20  0  0           1.000
   0 20 30  0           1.000
```

- Number of times to generate output using the zoom grid for concentration generation. The principle of using the zoom grid is explained in **??**. What essentially is done is to add the mass of all the particles in one grid cell of the zoom window and to calculate the concentration by dividing this mass by the volume of the cell. This is done for all cells in the zoom window (all layers).

Δ For every time, for which output using the zoom grid window is generated, 4 integers and 1 real must be provided. The integers specify the output times (in day, hour, minute, sec-

ond). The real gives the recovery factor. A recovery factor of 1.0 yields concentrations as modelled. A different recovery factor may be used to match the model results to measured data, if not all material is recovered with the measurements.

```
;                                Zoom grid output parameters
     5000.00      20000.00  ; x-start(m)              x-end(m)
    10000.00      25000.00  ; y-start(m)              y-end(m)
         150           150  ; grid cells in x dir(-)  grid cells in y dir(-)
```

- x-co-ordinates of the zoom window.
- y-co-ordinates of the zoom window.
  These values define the location and size of the zoom window. Output using the zoom grid output method will be limited to this window and if particle stray outside this window they will not be shown, even though these particles remain active in the model. The co-ordinates are all expressed in the same units as used in the hydrodynamic computation (for example national grid co-ordinates).
- Two numbers (integers) defining the number of grid cells in the x- and y-direction respectively.

```
;                      Instantaneous releases
    1  ; number of instantaneous releases

'dye release 1'
      0 12 30  0                          ; release time (dd hh mm ss)
        13210.00       17300.00       1 ; x-coord(m)     y-coord(m)      layer(-)
               0           0.00          ; option for release radius      radius[m]
                                         ; (0=user-defined radius;1=formula Fay-Hoult)
           50.00                         ; perc. of total particles(%)

;released mass(kg)
  1.000e+008        ; Tracer
      0.000         ; Tracer con 52
```

- Number of instantaneous releases.

Δ that many sets as instantaneous releases consisting of:

- a string containing the name of the release (at most 20 characters).
- 4 integers for the release time (day, hour, minute, second).
- 2 reals for the x- and y-co-ordinates of the release point (use the same co-ordinate system as the hydrodynamic grid).

$*$ (on the same line) one integer giving:

a for $K > 0$: the layer of the release. For dye releases the particles are uniformly distributed over the layer;

b for $K = 0$: a uniform release over depth.

- 1 integer to indicate if the radius is user-defined of calculated. Calculated is only possible for the oil model).

$\Delta*$ (on the same line) 1 real for the radius (in metres) of the release in the horizontal x, y-plane. Particles are uniformly distributed within this circle.

- 1 real specifying the percentage of the total number of particles that is going to be used to model the effects of this release. For instance, if you specified 10000 particles and a percentage of 50.0 for this release, than 5000 particles will be released at this (x, y)-co-ordinate (the mass corresponding to these particles must be specified below). The total percentages of all releases (inclusive the continuous releases) may be smaller or greater than 100 %, but in that case the number of particles released during the simulation will be less or more than the specified number of particles.
- for each substance the total mass that is going to be released (each values on a new line).

```
;                              Continuous releases
  1  ; number of continuous releases
```

```
'continuous release 1'
      13210.00       14000.00        3 ; x-coord(m)      y-coord(m)      layer
         0.000       50.00             ; radius(m)       perc. of total particles(%)
         1.000                         ; scale factor for load (kg/s)
             1                         ; interpolation option (0=block 1=linear)

; released_concentrations (kg/m3)
       0.000        ; Tracer
  1.000e+005        ; Tracer con 52

; release rates
 2
; dd hh mm ss     rate (m3/s)
   0 12 30  0         1.000
   0 20 30  0         1.000
```

- One integer giving the number of continuous releases.

Δ Define that many sets as continuous releases:

  - a string containing the name of the release (at most 20 characters)
  - 2 reals for the x- and y-co-ordinate of the release point.

  $*$ (on the same line) one integer K giving, specified in the same way as for instantaneous releases.

  - 1 real for the radius (in metres) of the release in the horizontal x, y-plane. Particles are uniformly distributed within this circle.

  $*$ 1 real specifying the percentage of the total number of particles that is going to be used to model the effects of this release.

  - 1 real for the required scale factor on a new line.
  - 1 integer to specify the interpolation option on a new line. A block function is specified by 0 and a linear interpolation by 1.
  - For each continuous release specify the concentrations of all tracers. The concentrations of the different tracers for a particular release are specified on a new line. The information for the different locations is on separate lines. The order of the locations is the same as the definitions of the releases.

- Now the mass to be released must be specified. This is done by means of specifying breakpoints that are either interpolated using a block function (0) or using a linear interpolation (1) — see the information on the interpolation option above.

  - An integer specifying the number of breakpoints.
  - For each breakpoint specify the time (days, hours, minutes, seconds) and the release rate. For each breakpoint, the time and release rate of all releases are specified on the same line.

```
;                           User defined releases
 0
```

- Instantaneous release or User-defined releases.
  This option is no longer supported and should be set to 0.

```
;                           Decay rates
 2
;dd hh mm ss          decay rates (1/day)
   0 12 30  0           0.000        0.000
   0 20 30  0           0.000        0.000
```

- one integer representing the number of "breakpoints" to specify the time variable decay coefficient. At least two breakpoints are required. Each record consists of the following:

Δ 4 integers giving the time of a breakpoint (day, hour, minute, second).

Δ as many reals (on the same line as the breakpoint specification) as there are substances, giving the first order decay coefficient per substance. The decay coefficient is assumed to be specified in [d^{-1}]. This information must be specified for at least two breakpoints. The

first breakpoint must be equal to the start time of the calculation, and the last breakpoint must be equal to the end time of the calculation.

```
;                            Settling velocities
; Generalized settling formula
          0.0000  ; exponent for c(-)
               1  ; grid refinement factor for accurate settling(-)

; Settling tables
            2  ; table dimension

; Tracer
; dd hh mm ss     A0[m/s]     A1[m/s]   Period[h]    Phase[h]   Vmin[m/s]   Vmax[m/s]
   0 12 30  0  1.000e-004       0.000       0.000       0.000     -10.000    1000.000
   0 20 30  0  1.000e-004       0.000       0.000       0.000     -10.000    1000.000

; Tracer con 52
; dd hh mm ss     A0[m/s]     A1[m/s]   Period[h]    Phase[h]   Vmin[m/s]   Vmax[m/s]
   0 12 30  0      0.000       0.000       0.000       0.000     -10.000    1000.000
   0 20 30  0      0.000       0.000       0.000       0.000     -10.000    1000.000
```

The time-variable settling velocities are specified in m/s.

- One real specifying the exponent for the concentration dependent settling (explained in **??**).
- The grid refinement factor (integer), used to calculate the concentrations needed to drive the concentration dependent settling velocity. The grid refinement factor is a multiplier of the number of grid cells in the x- and y-direction (see the box *Output Definitions*). If particles stray outside the zoom window, then the settling velocity will be set to 0.
- one integer representing the number of "breakpoints" for the time function for the (first order) decay coefficient.

  For each substance a block of data follows, specifying as many records as breakpoints. The following information should be present on each record:

△ 4 integers giving the time breakpoint (day, hour, minute, second).

△ four reals that specify the settling velocity: A_0 [m/s], A_1 [m/s], the period T [hours] and phase φ [hours], followed by the minimum and maximum allowable settling velocity. All values mentioned here are specified on the same line as the time of the breakpoint. For more information on the implementation of the time-variable settling velocities, see **??**.

```
;Sediment/erosion parameters
     5.0000e-002 ; Critical shear stress for sedimentation (Pa)
     4.0000e-001 ; Critical shear stress for erosion (Pa)
     5.5000e+001 ; Chezy coefficient (m1/2/s)
```

△ If the sedimentation/erosion option is switched on, the following constants must be given:

- Critical shear stress for sedimentation [Pa].
- Critical shear stress for erosion [Pa].
- Chézy coefficient [m$^{1/2}$/s].

Details of the sedimentation/erosion process are in **??**.

A.3 Oil module constants

In the previous section the Sub-datagroup Oil Model did not contain any parameters because the tracer model does not require any. When setting up the oil module, a number of specific oil module parameters are required. In the box below an example is given of a model with two oil types, three discharges for which the discharge radius of two discharges are calculated instead of using the supplied discharge radius as given in the instantaneous and continuous discharges boxes. For details of the model specific parameters see **??**.

```
;                            Oil model parameters
   22 ;number of constants
```

```
; Oil fraction dependent parameters
; Ekofisk
            0.4                ; Evaporation fraction per day
              1                ; Oil dispersion option [0/1]
                               ; (0=fraction per day 1=Delvigne/Sweeny formula)
              0                ; Sticky probability [0,1]
              1                ; Volatile fraction [0,1]
              0                ; Emulsification parameter C1
              1                ; Maximum water content C2  [0,1]
              1                ; Evap. fraction at which emulsification starts
            850                ; Density
             50                ; Kinematic viscosity
; Heavy Fuel Oil
           0.05                ; Evaporation fraction per day
              1                ; Oil dispersion option [0/1]
                               ; (0=fraction per day 1=Delvigne/Sweeny formula)
            0.5                ; Sticky probability [0,1]
           0.94                ; Volatile fraction [0,1]
         2e-006                ; Emulsification parameter C1
            0.7                ; Maximum water content C2  [0,1]
           0.05                ; Evap. fraction at which emulsification starts
            990                ; Density
           1500                ; Kinematic viscosity
; Global oil parameters
         5e-005                ; minimum thickness oil layer
              0                ; deflection angle (due to Coriolis force) - only for 3D
```

- an integer defining the number of model specific constants. For the oil module, this number will vary depending on a number of options that are selected within this input box.

Following the specification of the number of constants for this block, for each oil type a block of 8 parameters is specified (see section 5.5):

- the evaporation rate (per day).
- the choice of the formulation to calculate the oil dispersion (entrainment of oil in water). The options are:
  - 0 the dispersion is specified as a probability per day. The effect is an exponential reduction of surface floating oil.
  - 1 the Delvigne/Sweeney formulation for the oil dispersion (entrainment) is used, which means that the parameter that is specified is the kinematic viscosity [cSt].
  - $*$ the dispersed fraction per day (option 0) or the value of the kinematic viscosity of the oil (option 1).
- The probability of a particle to stick to the bottom or land boundary.
- The volatile fraction, i.e. the fraction of the oil that can evaporate.
- emulsification parameter C_1.
- Maximum water content (emulsification parameter C_2).
- Evaporated fraction at which emulsification starts.
- Density of oil.
- Kinematic viscosity of the oil.

Subsequent to the previous block follow some global oil parameters

- A real specifying the minimum oil layer thickness

Δ An integer specifying the deflection angle (in degrees, clockwise). This option is only applied in the 3D mode and for a 2DH model this parameter is not included in the input file.

A new setting not supported by the current GUI is a switch for sticking of oil at dry flats. To include it, you will have to changing the first line to version V3.73.00 or higher, and add the follow parameter, without increasing the number of constants:

```
  0                ; sticking at drying flats [0,1]
; (0=will not stick at dry flats, 1=will stick at dry flats)
```

A.4 Initial condition file for the oil module

The initial condition file (ASCII format) specifies one or more polygons that define surface oil patches. Each individual patch can be generated using QUICKIN, by creating a polygon file for each patch, for the file format see section A.5. If the polygon is not closed, then PART will close it by connecting the first and last co-ordinate of the polygon. More than one patch may be created. A header will then need to be added to each patch to specify the type and amount of oil for this patch and the number of particles associated with this patch. The type of oil will need to be the same as one of the oil types in the input file. An example of a initial conditions file is shown below.

```
*
*  Fraction:   Ekofisk
*  Mass:       1000000 kg
*  Particles:  10000
L00001
          13          2
   1.8809943E+05   6.1560469E+05
   1.8784460E+05   6.1639466E+05
   ...
   1.8860074E+05   6.1533856E+05
   1.8809943E+05   6.1560469E+05
*
*  Fraction:   Heavy Fuel Oil
*  Mass:       1000000 kg
*  Particles:  20000
L00002
          22          2
   1.9166405E+05   6.2069936E+05
   1.9486139E+05   6.2244163E+05
   ...
   1.9110883E+05   6.1937831E+05
   1.9166405E+05   6.2069936E+05
```

The keywords `Fraction`, `Mass` and `Particles` are compulsory. The $*$ at the beginning of the line is also required. These three keywords are then followed by a specification of the polygon name. The next line specifies the number of rows and number of columns that define the polygon, followed by the x, y data.

This $<*$.ini$>$ file can be visualised in the visualisation tool of the PART-GUI, by importing the file as a land boundary file.

In the input file the use of initial oil patches looks like:

```
 ;                           Initial condition (oil only)

               1 ; 0 = no initial particles
                 ; 1 = initial oil patches (from *.ini file)
 'ekofisk_hfo.ini' ; Initial condition file (including polygones describing the oil patches)
```

- An integer indicating if initial oil patches from a file are used.

Δ If for the oil module initial oil patches are required, then the name of this file is specified.

A.5 Polygon file

File contents	The co-ordinates of one or more polygons. Each polygon is written in a single block of data
Filetype	ASCII
File format	Free formatted
Filename	<*name*.pol>
Generated	RGFGRID, QUICKIN, D-WAQ DIDO, etc

Record description:

The file may contain one or more polygons. For every polygon the file should contain a line indicating the name of the polygon, followed by a line indicating the number of points making up the polygon and the number of coordinates, i.e. 2, finally followed by the coordinate data.

Record	Record description
	Preceding description records, starting with an asterisk ($*$), and will be ignored.
1	A non blank character string, starting in column one
2	Two integers representing the numbers of rows and number of columns for this block of data
	Two reals representing the x, y or λ, ϕ-coordinate

Restriction:

- ◇ The first record and the last record in the block should be the same

Example:

```
*
* Deltares, Delft3D-DIDO Version 3.39.01.4423:4459, Sep 25 2008, 20:10:54
* 2008-09-25, 22:11:08
*
Observation Area 001
       5   2
   1.8768018E+05   6.1708738E+05
   1.8996981E+05   6.1001035E+05
   1.9746314E+05   6.1266423E+05
   1.9480925E+05   6.1838830E+05
   1.8768018E+05   6.1708738E+05
Observation Area 002
       5   2
   2.0011703E+05   6.1818015E+05
   1.9819166E+05   6.1063479E+05
   2.0568498E+05   6.0870942E+05
   2.0797461E+05   6.1599460E+05
   2.0011703E+05   6.1818015E+05
Observation Area 003
       5   2
   1.9340425E+05   6.1396516E+05
   2.0183425E+05   6.1365294E+05
   1.9944054E+05   6.0558720E+05
   1.9522555E+05   6.0595146E+05
   1.9340425E+05   6.1396516E+05
```

A.6 Initial condition file for the oil module

The initial condition file (ASCII format) specifies one or more polygons that define surface oil patches. Each individual patch can be generated using QUICKIN, by creating a polygon file for each patch, for the file format see section A.5. If the polygon is not closed, then PART will close it by connecting the first and last co-ordinate of the polygon. More than one patch may be created. A header will then need to be added to each patch to specify the type and amount of oil for this patch and the number of particles associated with this patch. The type of oil will need to be the same as one of the oil types in the input file. An example of a initial conditions file is shown below.

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*  Mass:       1000000 kg
*  Particles:  10000
L00001
          13           2
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   1.8784460E+05   6.1639466E+05
   ...
   1.8860074E+05   6.1533856E+05
   1.8809943E+05   6.1560469E+05
*
*  Fraction:   Heavy Fuel Oil
*  Mass:       1000000 kg
*  Particles:  20000
L00002
          22           2
   1.9166405E+05   6.2069936E+05
   1.9486139E+05   6.2244163E+05
   ...
   1.9110883E+05   6.1937831E+05
   1.9166405E+05   6.2069936E+05
```

The keywords `Fraction`, `Mass` and `Particles` are compulsory. The $*$ at the beginning of the line is also required. These three keywords are then followed by a specification of the polygon name. The next line specifies the number of rows and number of columns that define the polygon, followed by the x, y data.

This <$*$.ini> file can be visualised in the visualisation tool of the PART-GUI, by importing the file as a land boundary file.

In the input file the use of initial oil patches looks like:

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- An integer indicating if initial oil patches from a file are used.

Δ If for the oil module initial oil patches are required, then the name of this file is specified.

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