

EMS: ENVIRONMENTAL MODELLING SUITE

SEDIMENT TRANSPORT MODULE

USER GUIDE



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1	INTRODUCTION	3
2	EMS STRUCTURE	3
3	SEDIMENT PROCESSES	4
4	INSTALLATION AND OPERATION	6
5	THE MODEL SET UP	6
6	GENERAL MECOSED PARAMETERS	6
6.1	Activate sediment module	6
6.2	Numerical grid	6
6.3	Skin roughness	7
6.4	Ripples	7
6.5	Bottom friction	8
6.6	Critical erosion stress	9
6.7	Critical deposition stresses	10
6.8	Flocculation	10
6.9	Consolidation	11
6.10	Biodiffusion	11
6.11	Initialisation diagnostic key	12
6.12	Maximum thickness of sediments	12
6.13	Wave input	12
6.14	Example	13
7	TRACER SPECIFIC PARAMETERS	14
7.1	MECOSED tracers	15
7.2	Initial concentrations	16
7.3	Settling velocity	17
7.4	Cohesive sediment	17
7.5	Resuspension deposition	17
7.6	Sediment grain density	17
7.7	Concentration of fresh sediment deposits	18
7.8	Flocculation key	18
7.9	Example of the tracer specific parameters	18
7.10	Sorption/desorption	19
7.11	Example for a sediment reactive tracer	19
7.12	Diagnostic files	20
8	BOUNDARY CONDITIONS	21
8.1	Example of a boundary condition	21
9	FILE INVENTORY	22
	REFERENCES	24

1 INTRODUCTION

EMS is a general-purpose modelling package that simulates three-dimensional flow, transport, and biogeochemical reactions in surface water. The model has been developed at CSIRO Marine and Atmospheric Division and tested and refined through a number of applications around the Australian coast. EMS comprises hydrodynamic, sediment transport and biogeochemical reaction modules.

Hydrodynamics of EMS is based on a 3-d nonlinear nonstationary hydrostatic approximation model SHOC (Herzfeld, 2008). The sediment model solves mass balance equations for sediment concentrations in a coupled benthic and pelagic layers taking into account bottom exchanges (Margvelashvili, 2008). Hydrodynamic and sediment models provide physical settings to biogeochemical model, which updates concentration of biogeochemical variables in water column and in sediments (Murrey and Parslow, 1997; Wild-Allen et al., 2005)

This report is designed to assist the user in operating sediment module of EMS. Theoretical and computational aspects of the sediment transport formulation are given in (Margvelashvili, 2003). Scientific background and application manual for EMS hydrodynamics can be found in (Herzfeld et al., 2002; Herzfeld and Waring, 2008).

2 EMS STRUCTURE

A general structure of EMS is illustrated in fig. 2.1. A 3-d hydrodynamic model is coupled to 1-d sediment transport model via a number of interface routines. During every simulation time-step these routines interrogate EMS (inquiring for hydrodynamic variables plus benthic data) to initialise the 1-d sediment model and to update forcing data. The sediment model then solves 1-d vertical advection-diffusion equations for every column of the numerical grid. Within every grid column the model solves equations for turbulent mixing in water column and bioturbation in sediments, and simulates sediment settling, erosion/deposition, and consolidation of sediments, plus vertical transport of the dissolved and sediment attached tracers. Updated profiles are stored in 3-d arrays of EMS representing benthic and pelagic layers. One way to think of the sediment module is that of a sewing machine coupling benthic and pelagic layers together in a single integrated system. Once the hydrodynamic and sediment transport steps are complete, EMS proceeds with the biogeochemical model updating concentrations of biogeochemical variables in benthic and pelagic cells.

When the sediment model is on, vertical diffusion and settling in a coupled benthic pelagic system is handled by the sediment model routines. The hydrodynamic model in this case simulates only horizontal diffusion and updates water velocities and 3-d advection of tracers in water column.

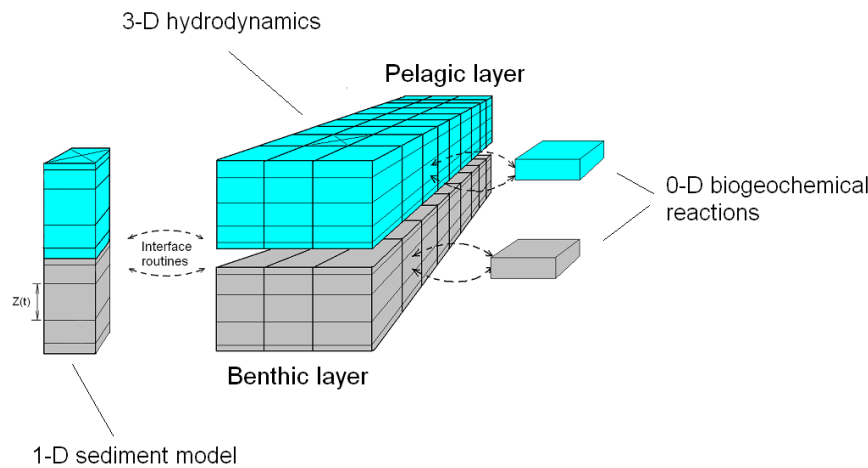


Fig. 2.1 Schematic structure of EMS

3 SEDIMENT PROCESSES

Sediment module of EMS is based on a 1-d vertical model of coastal and estuarine sediment transport - MECOSED (Margvelashvili, 2008). The model was intended as an improvement to the transport simulation capabilities of a 3-d coastal hydrodynamic/ water quality model MECO, developed at CSIRO, Division of Marine Research (Walker & Sherwood, 1997). MECOSED simulates vertical transport of particulate, dissolved, and sediment-bound tracers in water column and in sediment bed (Fig. 3.1).

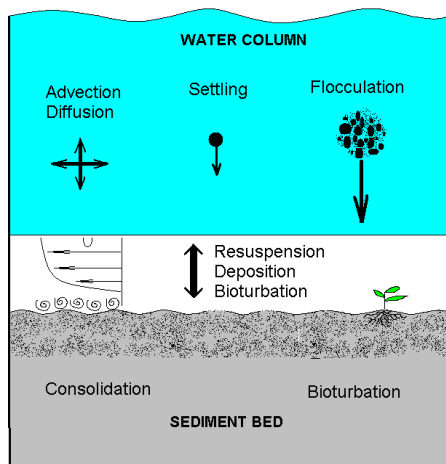


Fig. 3.1. Key sediment processes in MECOSED

Sediment transport

The sediment transport module of MECOSED solves advection-diffusion equations for the mass conservation of suspended and bottom sediments, taking into account bottom exchanges through the resuspension and deposition. Suspended particles undergo turbulent mixing and settling due to gravity force. Displacement of particles in sediment bed is driven by bioturbation and consolidation. The bioturbation is represented by local diffusion. Empirical formulas are used to parameterise sediment consolidation. Cohesive sediments are either eroded or deposited depending on

bottom shear stress and critical shear stress of the sediment resuspension and deposition. A concept of equilibrium sediment distribution is utilized to parameterize erosion/deposition of non-cohesive particles.

Dissolved transport

The module of the dissolved transport solves advection – diffusion equations of the mass conservation of tracers dissolved in water column and in sediment bed. Dissolved tracers undergo turbulent mixing in water column and diffusion in sediments. Transport in water is coupled with benthic processes through the diffusion across water and sediments and through the water entrainment/expulsion during resuspension/deposition or consolidation events.

Sediment-bound tracers

The sediment-bound tracer is analogous to a hydrophobic contaminant, e.g. organic chemical, heavy metal or radionuclide that adsorb to fine-grained sediment particles. The model solves advection – diffusion equations for the mass conservation of the sediment-bound tracers in water column and in sediment bed. Sorption exchange between solid and liquid phases is calculated using the concept of the equilibrium distribution. To simulate degradable pollutants, the model also incorporates first-order decay reaction.

Bottom boundary layer

Bottom friction under combined wave-current flow is calculated from bottom boundary layer model. On cohesive sediment bed constant physical roughness associated with biogenic bed-forms is specified. On non-cohesive sediment bed the total physical roughness is assumed to be composed of two components: one due to skin friction over the sediment grains and another due to form drag over the ripples. Ripples in a wave-dominated environment are either calculated or specified as the model input data. Under combined waves and currents and in a current-dominated flow the bed forms must be specified as the model input data.

Numerical solution

The numerical grid for sediment variables in the water column coincides with the numerical grid of the hydrodynamic model. Within the bottom sediments horizontal resolution of the model follows the resolution in water column. In vertical direction the model utilises stretched sediment-thickness-adapted grid which allows for high vertical resolution of the top sediments throughout the simulation.

The sediment model can run in a mode fully coupled to the hydrodynamic model and in a transport mode when the sediment transport is simulated off-line, using pre-calculated velocities and diffusion coefficients. The model benefits from high order numerical schemes developed in EMS. Curvilinear grids provide refined resolution in areas with high spatial gradients. The model capabilities also involve multiply nesting of the modelling domains (nested numerical grids), which gives a very high resolution in areas of a particular interest at a relatively low computational costs.

The developed model is particularly suitable for representing fine sediment dynamics.

4 INSTALLATION AND OPERATION

All installation and operation procedures required by the sediment module are covered by EMS installation requirements and can be found in SHOC user manual (Herzfeld and Waring, 2008).

5 THE MODEL SET UP

All input data for the sediment model are stored in a single ASCII parameter file. This file contains comments, key words, and values, and its contents completely describe a particular model implementation and run parameters. Data structure and parameter file format are exactly the same as used by the hydrodynamic module (Herzfeld and Waring, 2008). In a typical application the development of the sediment model follows the development of the hydrodynamic model. Throughout this document we assume that the hydrodynamic step is complete and parameter file of the hydrodynamic model is available (otherwise refer to SHOC manual describing the hydrodynamic model set up (Herzfeld and Waring, 2008)).

To set up the sediment model, the hydrodynamic model parameter file must be augmented with the sediment variables. The sediment data and parameters can be broadly classified into initialisation data, boundary data, parameters specific to a particular sediment tracer, and general sediment parameters. Detailed description of this data is given in the next chapter.

The output variables from the sediment module are handled by EMS infrastructure routines.

6 GENERAL MECOSED PARAMETERS

6.1 Activate sediment module

The sediment module of EMS is activated by adding the following command to EMS parameter file:

```
DO_SEDIMENTS 1
```

The default option is do not activate the sediment code:

```
DO_SEDIMENTS 0
```

6.2 Numerical grid

The numerical grid for sediment variables in the water column coincides with the numerical grid of the hydrodynamic model.

Numerical grid in sediments is defined by specifying initial thickness of every sediment layer in meters, starting from the top layer. An example of the sediment grid data is given below.

```
NSEDLAYERS      4
0.01
0.03
0.07
0.14
```

Here “NSEDLAYER” parameter gives the number of sediment layers, while the column underneath lists the thickness of each layer sequentially starting from the top layer. The top layer of the numerical grid represents an active layer of sediments and its thickness remains constant throughout the simulation. The thickness of the underlying layers varies with time in response to sediment resuspension/deposition and consolidation.

Constraints:

Numerical grid in sediments must include at least two sediment layers.

6.3 Skin roughness

Bottom skin roughness (in meters) associated with individual sediment grains is specified by

```
Z0_SKIN      0.00001
```

The value of the skin roughness can be estimated as a median grain size (~Nikuradze roughness height) divided by 30.

6.4 Ripples

Parameters PHYSRIPH, PHYSRIPL prescribe the ripple height and length (in meters) on sandy sediments, respectively. The development of such ripples is associated with the physical processes (waves and currents). The BIORIPH and BIORIPL parameters provide dimension of ripples on a cohesive seabed, where ripples development is typically associated with the biological reworking of the benthic layer.

```
PHYSRIPH      0.02
PHYSRIPL      0.6
BIORIPH       0.005
BIORIPL       0.2
```

Unless the ripple dimension is simulated, the model takes the largest out of the PHYSRIPH and the BIORIPH as a representative ripple height and the largest out of the PHYSRIPL and the BIRIPL as a representative ripple length.

Once the ripple dimension is specified, MECOSSED proceeds with estimating bottom roughness due to ripples according to Grant and Madsen (1982) formula.

In a wave dominated environment simulation of the ripple dimension can be activated by

`CALC_RIPPLES 1`

In this case the model estimates the ripple height and length based on Wakramanayake (1993) model. Ripples are estimated only over sandy sediments. On a cohesive bed ripple dimension is specified as an input data from the parameter file (see description of BIORIPH and BIORIPL parameters above).

The default option for estimating ripples is do not estimate the ripple dimension:

`CALC_RIPPLES 0`

In this case the ripple dimension must be specified in a parameter file.

Constraints:

An option for ripple calculation “CALC_RIPPLES 1” has never been used in our case studies and remains largely untested. We recommend to use “CALC_RIPPLES 0” and have the ripple dimension prescribed as the model input data.

6.5 Bottom friction

Two options are available in MECOSSED to estimate bottom friction. One is based on nonlinear Grant and Madsen model (Madsen 1994), which is activated by

`BBL_NONLINEAR 1`

The model requires wave/current data and bottom roughness as an input. The bottom roughness is computed as a sum of the skin roughness and the roughness due to ripples (see section 6.4). The wave/current data must be provided from the hydrodynamic module.

An alternative option for calculating bottom friction is based on a linear bottom boundary model activated by

`BBL_NONLINEAR 0`

With this option the bottom friction is approximated as a sum of the current friction over the ripples and the wave friction over the sediments grains. There is no interaction between waves and currents. The bedform roughness is used to estimate friction of currents over the ripples, and the skin roughness is used to estimate wave friction over the individual sediment grains.

The default option for bottom boundary layer model is Grant and Madsen model:

BBL_NONLINEAR 1

6.6 Critical erosion stress

Five options (CSS0, CSS1, CSS2, CSS3, CSS4) are available in MECOSSED to estimate critical shear stress on a cohesive sediment bed. A particular option can be specified using the key CSS_ER_MODE. An example is given below.

```
CSS_ER_MODE    CSS0
```

The simplest CSS0 mode assumes constant critical shear stress. The value of this constant can be specified as

```
CSS_ER 0.25
```

The default value of the critical erosion stress is 0.2 (N/m²).

In CSS1, CSS2, CSS3 modes critical shear stress is calculated as a function of the sediment bed compactness using empirical formulations (5.5), (5.6), and (5.7), respectively (see MECOSSED scientific manual). Note that CSS1-3 options typically imply that the sediment porosity varies with time due to consolidation processes.

An option CSS4 specifies the critical shear stress of erosion that varies with the sediment depth. The shear stress values must be specified using the key CSS_ER. An example is given below

```
CSS_ER 4
0.2
0.3
0.5
0.7
```

The corresponding depth levels (in m) are given by the key CSS_ER_DEPTH:

```
CSS_ER_DEPTH 4
-0
-0.002
-0.1
-0.2
```

In this example the critical shear stress of erosion is 0.2 N m⁻² for sediments allocated below 0 and above 0.002 m depth. The critical shear stress is 0.3 for sediments below 0.002 and above 0.1 m depth, and so on. Note that the number following CSS_ER and CSS_ER_DEPTH keys now specifies the number of the sediment layers with a distinct critical shear stress value.

Critical erosion stress for non-cohesive sediments is calculated as a quarter of the sediment settling velocity. The reference height for the reference velocity is specified at seven Nikuradze roughness heights (7*30* Z0_SKIN).

Constraints:

CSS1-3 options have never been tested in real world applications. An option CSS0 or CSS4 is recommended.

6.7 Critical deposition stresses

Critical shear stress of cohesive sediment deposition (in N/m^2) is given by

```
CSS_DEP      0.3
```

In a default mode cohesive sediments are always allowed to settle on the sediment bed, e.g. $\text{CSS_DEP} = +\text{inf}$.

6.8 Flocculation

A number of options is currently available in MECOSSED to calculate cohesive sediment flocculation (FLOC0, FLOC1, FLOC4). A particular option is specified by the key FLOC_MODE:

```
FLOC_MODE    FLOC0
```

The simplest FLOC0 mode assumes that sediments do not flocculate. FLOC1 mode predicts mean floc velocities as a function of cohesive sediment concentration. FLOC2 and FLOC3 modes are under construction and currently are not available. FLOC4 mode is based on empirical formulation for settling velocity of cohesive sediment derived from observations in the Brisbane estuary. The default mode is FLOC0, i.e. sediments do not flocculate.

If the flocculation mode FLOC1 is on:

```
FLOC_MODE    FLOC1
```

two additional parameters must be specified

```
FLOC_PRM1  1.  
FLOC_PRM2  2.
```

Here FLOC_PRM1 is a scaling parameter and FLOC_PRM2 is a power of the exponential term in a power law approximation of the sediment flocculation (see formula (5.2) in the MECOSSED science manual).

An option

```
FLOC_MODE    FLOC4  
FLOC_PRM1  2e-4
```

makes the model to estimate settling velocity of the sediment flocs using an empirical relationship based on observations in the Brisbane estuary and Moreton Bay (see

formula 5.4 in the MECOSSED science manual). The parameter FLOC_PRM1 in this case represents settling velocity of the individual sediment grains in (m s⁻¹).

All flocculation modes involve scaling of the settling velocity by the water salinity, so that there is no flocculation when the water salinity is less than 0.1 ppm. The flocculation of a particular sediment fraction is controlled by additional tracer-specific parameter TRACER#.floc which is described in section 7.8.

Constraints:

FLOC1 and FLOC4 options require salinity to be included in the list of the hydrodynamic model variables.

6.9 Consolidation

Consolidation of sediments is activated by

CONSOLIDATE 1

If this indicator is on then the model requires also data on final minimal porosity of sediments (FINPOR_SED, non-dimensional), and typical time scale of the sediment bed consolidation (CONSOLRATE, in days):

FINPOR_SED	0.3
CONSOLRATE	5.e+0

The default option is no consolidation:

CONSOLIDATE 0

Constraints:

We have never used consolidation option in our case studies. An option “CONSOLIDATE 0” is recommended.

6.10 Biodiffusion

Biological activity of the benthic layers is given by the parameter

BIODENS	100.0
---------	-------

which prescribes the number of standard animals per square metre of sediments.

Maximum depth for the biological activity (in meters) is specified as

MAXBIODEPTH	0.2
-------------	-----

Diffusion coefficients for bio-turbation (BT_PARTIC_KZ, in m²/s) and bio-irrigation (BI DISSOL_KZ, in m²/s) of sediments are scaled by the amount of biological activity present (m²/s per animal/m²), and also decrease with depth in sediment bed

according to some fixed profile. Diffusion coefficients in the sediment bed are specified as follows

BI DISSOL_KZ 1.0e-10
BT PARTIC_KZ 1.0e-10

Diffusion coefficients across sediment – water interface are given by

BI DISSOL_KZ_I 1.0e-12
BT PARTIC_KZ_I 1.0e-12

Functional form of the scaling profile for bioirrigation and bioturbation activity as a function of depth is prescribed by one of the following strings: constant, linear, parabolic, gaussian:

BIOSEDPROFILE parabolic

6.11 Initialisation diagnostic key

The key

VERBOSE_SED 1

downloads “sedlog.txt” file containing sediment initialisation diagnostics. The default option is no diagnostics.

6.12 Maximum thickness of sediments

The maximum thickness of sediments can be specified by

MAX_THICK_SED 2

There is no feedback in EMS from the sediment processes to the hydrodynamic model, so that any changes in the sediment thickness do not translate into the corresponding changes of the water depth. An implicit assumption underlying this approximation is that changes in the sediment thickness are small compared to the water depth. This assumption can be violated particularly during long-term simulations. To avoid unrealistic situations where the sediment thickness exceeds the water depth we introduce the parameter MAX_THICK_SED. Sediment particles are not allowed to settle on the seabed in areas where the sediment thickness has reached the maximum predefined value.

6.13 Wave input

Wave input is represented by the amplitude of the near bottom wave orbital velocities (m s⁻¹), wave period (s) and wave direction (degrees). The direction angle is given as

degrees Cartesian referenced to the West-East direction counter-clockwise. The wave data are updated at time intervals given by WAVE_VARS_INPUT_DT:

```
WAVE_VARS_INPUT_DT 1 hour
```

The wave-data source-file is specified through the key WAVE_VARS:

```
WAVE_VARS          waves.nc
```

The default option is no waves.

6.14 Example

Example of EMS parameter-file section that specifies general parameters of the sediment model is given below.

```
#####  
#####  
# Sediments  
  
VERBOSE_SED 1  
  
# Sediment layers thickness  
NSEDLAYERS 3  
0.005  
0.015  
0.19  
  
# Activate sediment process  
Default: 0  
DO_SEDIMENTS 1  
  
# CRITICAL STRESSES  
# Critical shear stress of cohesive bed erosion (N m-2)  
# Modes: CSS0, CSS1, CSS2, CSS3  
# Default: CSS0: css_er = 0.2  
CSS_ER_MODE CSS0  
CSS_ER 0.05  
  
# Critical shear stress of cohesive sediment deposition (N m-2)  
# Default: CSS_DEP = +inf  
#CSS_DEP 0.3  
  
# FLOCCULATION  
# Modes: FLOC0, FLOC1  
# Default: FLOC0 - no flocculation  
FLOC_MODE FLOC1  
FLOC_PRM1 300  
FLOC_PRM2 3  
  
# CONSOLIDATION  
CONSOLIDATE 0  
FINPOR_SED 0.4  
CONSOLRATE 10.e+0
```

```

# Bottom Boundary Layer model
BBL_NONLINEAR 1

# Bottom Skin roughness (m)
Z0_SKIN 0.00003

# RIPPLES
# Default: 0
PHYSRIPH 0.03
PHYSRIPL 0.6
BIORIPH 0.005
BIORIPL 0.2

# Maximum depth for biological activity (m)
MAXBIODEPTH 0.2

# Functional form for bioirrigation and bioturbation activity
# as a function of depth. Currently can be one of:
#   constant
#   linear
#   parabolic
#   gaussian
# Only the first letter of this parameter is significant
BIOSEDPROFILE parabolic

# Biological activity (standard animals per square metre?)
BIODENS 10.0

# Diffusion coefficient for bio-irrigation of sediments.
# This value is scaled by the amount of biological
# activity present, and also decreases with depth
# in the sediment according to some
# fixed profile. The value here is the value which
# would apply at zero depth in the sediment.
# Units are m2 s-1 per animal per m2.
BI DISSOL_KZ 1.0e-9
BI DISSOL_KZ_I 1.0e-9

# Diffusion coefficient for bio-turbation of sediments.
# This value is scaled by the amount of biological
# activity present, and also decreases with depth
# in the sediment according to some
# fixed profile. The value here is the value which
# would apply at zero depth in the sediment.
# Units are m2 s-1 per animal per m2.
BT PARTIC_KZ 1.0e-10
BT PARTIC_KZ_I 1.0e-12

#####
#####
# Activate Waves
DO WAVES YES
WAVES_DT 1 hour
WAVE_VARS YES
#WAVES BOT_STRESS VERT_MIX

```

7 TRACER SPECIFIC PARAMETERS

Apart from the general model parameters each tracer of EMS has its own set of the tracer specific parameters. A general guideline for tracer specification in EMS can be found in (Herzfeld and Waring, 2008). This chapter describes tracer parameters specific to MECOSED.

7.1 MECOSED tracers

MECOSED calculates transport of two basic types of tracers: particulate and dissolved (fig 7.1). Particulate tracers represent either volumetric particles or zero-volume tracers. Volumetric particles settle due to gravity force and change porosity in water column and in sediment bed. The concentration of volumetric particles is limited by free volume available in water column or in sediment bed.

Zero-volume particles are assumed to occupy zero volume in space. A typical example of zero-volume tracer is a sediment-attached tracer (pollutant). As any particulate tracer the sediment-attached tracer undergoes settling and resuspension/deposition in water column and bioturbation/consolidation in sediments but unlike to sediments it does not change porosity of the sediment layer.

It is recommended to treat also biogeochemical reaction variables as zero volume tracers, so that any transient instabilities in biogeochemical model simulations do not blow away the sediment layer.

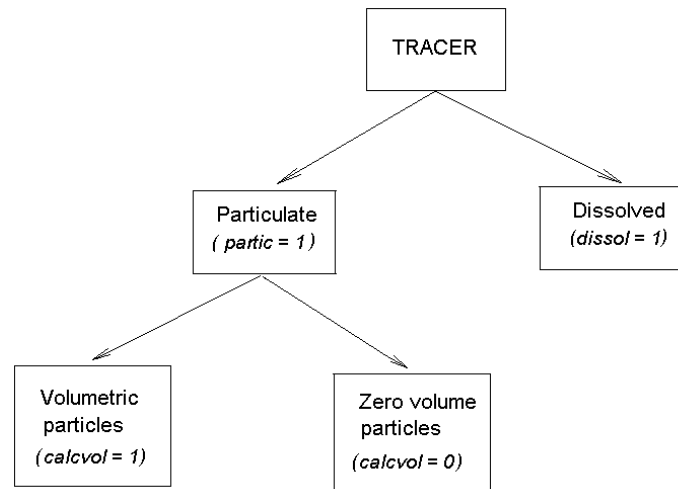


Fig. 7.1 MECOSED tracers

Every MECOSED tracer must be specified as either particulate tracer

TRACER4.partic 1

or dissolved tracer

TRACER4.dissol 1

The volumetric tracer can be specified using the following string:

```
TRACER4.calcvol 1
```

Default value for “calcvol” is zero and the tracer is considered as having zero volume of constituting particles. If the flag calcvol is on (volumetric tracer) then the tracer is not allowed to attach to any sediment fraction (adsorb = 0).

7.2 Initial concentrations

Initial concentration of each sediment fraction is specified individually for each tracer in a tracer description file. To indicate that a particular tracer is present in both water column and sediments, a type indicator must be added to the tracer description list

```
TRACER#.type WATER SEDIMENT
```

Then the concentration units are specified by

```
TRACER#.units kg m-3
```

This is followed by valid range of the concentrations in water and in sediments

```
TRACER#.valid_range_wc 0 1000
```

```
TRACER#.valid_range_sed 0 3000
```

Finally the initial concentrations of the tracer in water and in sediments is specified by

```
TRACER#.fill_value_wc 0.01
```

```
TRACER#. fill_value_sed 600
```

Spatially varying fields of the initial sediment deposits can be specified through the interpolation of observations. Observations must be stored in an ASCII file (for instance init_deposit.txt file) with the first and second columns representing longitude and latitude of the sampling site respectively and the rest columns showing observed concentrations.

```
TRACER#.data_sed      init_deposit.txt
```

```
TRACER#.interp_type  linear
```

The data file format is the same as that used for boundary data (see section 8.1). The interpolation type is given by the key TRACER#.interp_type.

Constraints:

If the concentration units for sediments and dissolved tracers differ from “kg m⁻³” then the model assumes that the concentration is given in “mg m⁻³” (except for sediment attached pollutants). Concentration of the sediment-attached tracers must be given as some activity per unit volume (Activity m⁻³) rather than per unit mass.

It is recommended to keep initial concentration of all sediment fractions within the reasonable bounds so that to insure that initial porosity of sediments exceeds 0 but is lower than 1.

Benthic layer of MECOSSED must always include some sediment particles. In applications with a high-energy environment it is recommended to include in MECOSSED a sediment class

representing heavy particles (eg gravel fraction) that would form a baseline un-erodible substrate underlying fine sediments.

EMS typically does not resolve bed-load transport layer. Z-coordinate grids produce step like representation of bathymetry. Hence, the developed 3-d sediment module is particularly suitable for simulating transport of only fine sediments.

If the sediment flocculation is on, the salinity field must be specified in both benthic and pelagic layers (eg. `TRACER#.type WATER SEDIMENT`).

7.3 Settling velocity

Settling velocity of the particulate tracer is given by

```
TRACER4.svel -0.001
```

Default is 0.

This parameter specifies settling velocity of the individual sediment grains. When sediments flocculate the settling velocity of the flocs is estimated through the flocculation model and the largest of the two (the settling velocity of the individual grains and the settling velocity of the flocs) is used to settle sediment particles.

7.4 Cohesive sediment

MECOSED employs two different formulations for sediment resuspension on cohesive and non-cohesive sediment bed. A particular sediment resuspension regime could be specified by assigning zero (non cohesive) or unit (cohesive) value to “cohesive” flag:

```
TRACER4.cohesive 1
```

Default value is cohesive.

7.5 Resuspension deposition

Resuspension and deposition of any particular tracer is controlled by “resuspend” and “deposit” flags:

```
TRACER4.resuspend 1  
TRACER4.deposit 1
```

Default is resuspend and deposit. If both “resuspend” and “deposit” flags are off, then there is neither resuspension nor deposition of particles across water and sediments. Note that unless diffusion fluxes across water and sediments is switched off (see section on 6.10 on Biodiffusion), benthic and pelagic layers in this case are not fully decoupled.

7.6 Sediment grain density

Density of sediment grains (kg/m³) is specified by

```
TRACER4.b_dense 2.65e+03
```

The sediment grain density (along with the mass concentration and the grid cell volume) is used to calculate the seabed porosity.

7.7 Concentration of fresh sediment deposits

Concentration of fresh sediment deposits (kg/m³) is given by

```
TRACER4.i_conc 1.2e+03
```

This parameter is used to estimate the volume of water trapped in sediments during the deposition event.

7.8 Flocculation key

Flocculation of individual tracers can be switched on or off with the following flag

```
TRACER4.floc 1
```

Default is 0 (no flocculation).

7.9 Example of the tracer specific parameters

This section shows an example of the tracer specifications for sediment particles

```
TRACER4.name Silt
TRACER4.long_name Silt fraction
TRACER4.type WATER SEDIMENT
TRACER4.units kg m-3
TRACER4.valid_range_wc 0 1e+35
TRACER4.valid_range_sed 0 1e+35
TRACER4.diagn 0
TRACER4.fill_value_wc 0.0
TRACER4.fill_value_sed 600.0
TRACER4.dissol 0
TRACER4.partic 1
TRACER4.advect 1
TRACER4.diffuse 1
TRACER4.decay 0
TRACER4.b_dens 2.65e+03
TRACER4.i_conc 1.2e+03
TRACER4.svel -0.2e-3
TRACER4.cohesive 1
TRACER4.calcvol 1
TRACER4.floc 1
TRACER4.resuspend 1
TRACER4.deposit 1
```

7.10 Sorption/desorption

Any particulate (partic 1) zero-volume (calcvol 0) tracer in MECOSSED can be attached to any other particulate (partic 1) volumetric (calcvol 1) tracer by specifying “adsorb” flag (1 if adsorbed, 0 if not adsorbed).

```
TRACER4.adsorb 1
```

and indicating the name of the sediment class carrying this particular adsorbed tracer

```
TRACER4.carriename Clay
```

The above strings indicate that the tracers N4 is attached (adsorbed) to the tracer called “Clay”. The tracer “Clay” must represent some particulate volumetric tracer.

To simulate sorption/desorption exchange between particulate and dissolved fractions of the sediment reactive tracer, the user ought to indicate the corresponding dissolved fraction and specify sorption parameters.

The dissolved fraction of the sediment reactive tracer is identified by the parameter “dissolvedname” indicating the name of the dissolved tracer:

```
TRACER4.dissolvedname ZincDis
```

The above strings indicate that the sediment reactive tracer N4, attached to the sediment tracer “Clay”, has the dissolved counterpart “ZincDis”.

An equilibrium distribution constant for the desorbed and adsorbed fractions of the sediment reactive tracer is specified by the parameter “adsorbkd” (in m³/kg)

```
TRACER4.adsorbkd 20
```

And the adsorption rate constant (in days) is given by

```
TRACER4.adsorbrate 1
```

MECOSSED employs first order kinetic reaction to simulate sorption/desorption reactions between particulate and dissolved fractions of the sediment reactive tracer (equations 7.3, 7.4, MECOSSED science manual). Note that concentrations of the sediment reactive tracers are given as an activity per unit volume, rather than per unit mass.

7.11 Example for a sediment reactive tracer

This section gives an example of the tracer specifications for the sediment reactive tracer.

```
TRACER6.name ZNclay
TRACER6.long_name Zn on clay
TRACER6.type WATER SEDIMENT
```

```

TRACER6.units g m-3
TRACER6.valid_range_wc 0 1e+35
TRACER6.valid_range_sed 0 1e+35
TRACER6.diagn 0
TRACER6.fill_value_wc 0.0
TRACER6.fill_value_sed 0.0
TRACER6.dissol 0
TRACER6.partic 1
TRACER6.advect 1
TRACER6.diffuse 1
TRACER6.b_dens 2.65e+03
TRACER6.i_conc 1.2e+03
TRACER6.decay 0
TRACER6.adsorb 1
TRACER6.carriername Clay
TRACER6.dissolvedname ZincDis
TRACER6.adsorbkd 20
TRACER6.adsorbrate 1

```

7.12 Diagnostic files

A number of 3d and 2d diagnostic variables specific to sediment processes can be added to the stream of the model output by specifying extra diagnostic tracers in the parameter file. The diagnostic tracer is identified by the key (TRACER#.diagn 1).

The 3d diagnostic variables specific to sediments are

“tss”: total suspended sediment concentration in water and in sediments,
“svel_floc”: settling velocity of the sediment flocs in water column, and velocity of consolidating particles in sediments;
“porosity”: porosity in water and porosity in sediments;
“cohسد”: cohesive sediment fraction given as a mass percentage of cohesive sediments relative to the total mass of either suspended or bottom sediments.

A particular 3-d variable is identified by its name (for example “tss”). Note that the sediment settling velocity is estimated in the model as the largest of the settling velocity of individual grains and the settling velocity of flocs, so that if there are no flocs present (svel_floc = 0) sediments still settle due to gravity force acting on the individual sediment grains. Porosity in water column is always assumed to be equal to 1.

All 3d diagnostic variables must be specified as of WATER SEDIMENT type.

2d diagnostic variables include:

“ustrew_skin” bottom shear stress velocity (m s-1)
“depth_sed” sediment thickness (m)
“dzactive” thickness of the top active layer of sediments (m)
“hripple” ripple height (m)
“lripple” ripple length (m)

All 2d diagnostic variables must be specified as of BENTHIC type.

An example bellow illustrates specification of the 3d and 2d diagnostic variables:

```
TRACER7.name tss
TRACER7.long_name tss
TRACER7.type WATER SEDIMENT
TRACER7.units kg m-3
TRACER7.valid_range_wc 0 1e+35
TRACER7.valid_range_sed 0 1e+35
TRACER7.fill_value_wc 0.0
TRACER7.fill_value_sed 0.0
TRACER7.advect 0
TRACER7.diffuse 0
TRACER7.diagn 1
```

```
TRACER8.name ustrcw_skin
TRACER8.long_name ustrcw_skin
TRACER8.type BENTHIC
TRACER8.units m s-1
TRACER8.valid_range_wc 0 1e+35
TRACER8.valid_range_sed 0 1e+35
TRACER8.fill_value_wc 0.0
TRACER8.fill_value_sed 0.0
TRACER8.advect 0
TRACER8.diffuse 0
TRACER8.diagn 1
```

An extra diagnostics can be inferred from the model output through the development of customised processing scripts interrogating netcdf files produced by the model (tracers in sediments in the output files are identified by suffix “_sed” added to the tracer name).

8 BOUNDARY CONDITIONS

MECOSED assumes no sediment fluxes through the water surface, at the bottom of the benthic layer, and at the lateral land boundaries. To specify sediment concentrations at the open sea lateral boundaries, data file must be provided and referenced to in the list of the boundary condition specifications. For more details on open boundary specification for tracers please refer to SHOC manual (Herzfeld and Waring, 2008)

8.1 Example of a boundary condition

This section includes an example of the boundary conditions for hydrodynamic and sediment variables at the open sea boundary. Features relevant to MECOSED are highlighted in bold. The parameters “**BCOND_TRA3**” and “**BCOND_TRA4**” indicate that the boundary data for tracer 3 and tracer 4 are specified in data files. The location of this data file “**bnd_ocean.ts**” is indicated by the 3rd highlighted line.

```
BOUNDARY0.NAME north
BOUNDARY0.TYPE u1
BOUNDARY0.BCOND_NOR CUSTOM
BOUNDARY0.CUSTOM.u1 uv_to_u1
/home/mgdata/dent/c2_mgs/run6_coarse_uv_n.nc
BOUNDARY0.BCOND_TAN CLAMPD
```

```

BOUNDARY0.CUSTOM.u2    uv_to_u2
/home/mgdata/dent/c2_mgs/run6_coarse_uv_t.nc
BOUNDARY0.BCOND_ELE    NOTHIN
BOUNDARY0.BCOND_TRA_ALL NOGRAD
BOUNDARY0.BCOND_TRA0   FILEIN
BOUNDARY0.BCOND_TRA1   FILEIN
BOUNDARY0.BCOND_TRA2   NOGRAD
BOUNDARY0.BCOND_TRA3   FILEIN|UPSTRM
BOUNDARY0.BCOND_TRA4   FILEIN|UPSTRM
BOUNDARY0.BCOND_VZ     NOGRAD
BOUNDARY0.BCOND_KZ     NOGRAD
BOUNDARY0.DATA         /home/mgproja/dent/st_meco/ctd_station1.nc
/home/mgproja/sedi_mgf/huon/3d/bnd_ocean.ts
BOUNDARY0.INVERSE_BAROMETER FALSE
BOUNDARY0.POINTS      2
53 12
53 13

```

An example of the open sea boundary data file (“bnd_ocean.ts”) is given below.

```

## COLUMNS 3
##
## COLUMN1.name Time
## COLUMN1.long_name Time
## COLUMN1.units days since 2001-06-01 00:00:00 +10
## COLUMN1.missing_value -999
## COLUMN1.fill_value 0.0
##
## COLUMN2.name Sand
## COLUMN2.long_name Sand
## COLUMN2.units kg s-1
## COLUMN2.missing_value -999
## COLUMN2.fill_value 35
##
## COLUMN3.name Silt
## COLUMN3.long_name Silt
## COLUMN3.units kg s-1
## COLUMN3.missing_value -999
## COLUMN3.fill_value 35
##
-1e13 0.0 0.01
1e13 0.0 0.01

```

9 FILE INVENTORY

The sediment model file inventory is shown in table 9.1.

N	Filename	Description
1	sed_init.c	MecoSed initialisation routine.
2	Hyd2sed.c	Data flow from EMS to mecosed
3	Sed2hyd.c	Data flow from mecosed to EMS
4	Bbl.c	Bottom boundary layer model
5	Vtransp.c	Vertical transport in water column and sediment bed
6	Trvdifsettl.c	Implicit vertical diffusion, settling, erosion/deposition.
7	sediments.c	Sediment step file

8	Sediments.h	Include file for mecosed structures
---	-------------	-------------------------------------

Table 9.1 MECOSED file inventory

REFERENCES

Herzfeld, M., Waring, J., Parslow, J., Margvelashvili, N., Sakov, P., Andrewartha, J., 2008. SHOC: Sparse Hydrodynamic Ocean Code Science manual. CSIRO internal document. 121 p.

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Margvelashvili, N., 2003. "MECOSED – Model for Estuarine and Coastal Sediment Transport, Scientific Manual", CMAR internal document, 46 p.

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