EMS: ENVIRONMENTAL MODELLING SUITE

SEDIMENT TRANSPORT MODULE

USER GUIDE



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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, 2016).

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 first the hydrodynamic model updates 3D hydrodynamic fields. The interface routines interrogate EMS (inquiring information about updated state variables in water column and in sediment bed) to initialise 1-d sediment transport model then solves 1-d vertical advection-diffusion equations for every dissolved and particulate tracer. 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. Having the hydrodynamic and sediment transport steps complete, EMS proceeds with the biogeochemical model updating concentrations of biogeochemical variables in benthic and pelagic cells.



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 formulation is 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 entrainment/expulsion of water attached to sediment particles during resuspension and deposition events. Dissolved tracers can also cross the sediment/water interface during the consolidation of sediments which expel pore water into the pelagic system.

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 sediment 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 wavedominated 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 transport model can be fully coupled to the hydrodynamic model implying that both models run in parallel and have the same time step. The alternative option is to simulate sediment transport in off-line mode. In this case currents and diffusion coefficients saved from the hydrodynamic model run provide inputs into the stand-alone sediment transport model. The simulation time-step is much larger than that of the coupled model and there is no feedback from the sediment processes to the

hydrodynamics, i.e. the impact of sediments on flow, density and turbulence are not simulated. This decoupling of the sediment and hydrodynamic models provided substantial benefits in computational efficiency, and is implemented for the eReefs sediment transport models.

The sediment transport 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, 2016).

5 THE MODEL SET UP

All input parameters of the sediment model are stored in a single ASCII parameter file. This file contains comments, key words, and values, and its content provides complete description of a particular implementation of the model and its run-time parameters. For a fully coupled hydrodynamic, sediment-transport models the structure of input data and a parameter-file format are exactly the same as that used by the hydrodynamic module (Herzfeld and Waring, 2016). For an offline simulation of the sediment transport, a lightweight version of the parameters file (called a transport parameter-file and typically named as *.tran) is required. This transport parameter-file describes location of hydrodynamic forcing files, specifies parameters specific to the transport mode of simulation, and also defines parameters of the sediment transport model. 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 either a parameter file of the hydrodynamic model or a transport parameter-file specifying dispersion of a dissolved tracer is already available (otherwise refer to SHOC manual describing the hydrodynamic model set up (Herzfeld and Waring, 2016)).

To run the sediment transport model fully coupled to the hydrodynamic model, the hydrodynamic model parameter-file must be augmented with parameters specific to the sediment transport model. Analogously, to simulate sediment transport off line, the transport parameter-file must be augmented with the sediment model parameters.

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 sections of this document. 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 provides 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 underlaying layers varies with time to either accommodate new deposits or expel porewater in consolidating sediments.

Comments:

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 benthic layers.

0.02
0.6
0.005
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, MECOSED proceeds with estimating bottom roughness due to ripples according to Grant and Madsen (1982) formula.

In a wave dominated environment simulation of ripple dimensions 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 ripple dimensions:

CALC_RIPPLES 0

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

Comments:

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 MECOSED 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

In this case the bottom friction is evaluated 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 the 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 MECOSED 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 MECOSED 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 above the initial surface of sediments (0 m depth). The critical shear stress is 0.3 for sediments above 0.002 m but below 0 m depth, and so on. The number on the same line as CSS_ER and CSS_ER_DEPTH keys specifies the number of 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/m²) is given by

CSS_DEP 0.3

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

6.8 Flocculation

A number of options is currently available in MECOSED 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 low approximation of the sediment flocculation (see formula (5.2) in the MECOSED 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 MECOSED science manual). The parameter FLOC_PRM1 in this case represents settling velocity of an individual sediment grain 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.

Comments:

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_SED0.3CONSOLRATE5.e+0

The default option is no consolidation:

CONSOLIDATE 0

Comments:

Consolidation has never been tested through our regular case studies. An option "CONSOLIDATE 0" is recommended.

6.10 Biodiffusion

Bioturbation and bio-irrigation processes in sediments are represented by diffusion of particulate and dissolved tracers across benthic layers. Diffusion within sediments is parameterised by diffusion coefficients for the bioturbation (BT_PARTIC_KZ) and bio-irrigation (BI_DISSOL_KZ), both given in (m²/s). For example:

BI_DISSOL_KZ 1.0e-10 BT_PARTIC_KZ 1.0e-10

Analogously, diffusion across sediment – water interface is parameterised by the corresponding diffusion coefficients for the dissolved and particulate tracers (in m^2/s)

BI_DISSOL_KZ_I 1.0e-12 BT_PARTIC_KZ_I 1.0e-12

An intensity of both bioturbation and bio-irrigation is scaled by the number of standard animals per square metre of sediments (animal/ m^2)

BIODENS 100.0

Maximum sediment depth for a biological activity is specified in meters

MAXBIODEPTH 0.2

Functional form of the scaling profile for the bio-irrigation and bioturbation processes as a function of depth is given by one of the following keys: constant, linear, parabolic, gaussian. For example:

BIOSEDPROFILE parabolic

6.11 Initialisation diagnostic key

The key

VERBOSE_SED 1

downloads "sedlog.txt" file containing sediment initialisation and run-time diagnostics. The default option is no diagnostics.

Comments: Beware of verbose sediments producing extremely large files accumulating with time.

6.12 Maximum thickness of sediments

The maximum thickness of sediments (in meters) can be specified by

MAX_THICK_SED 2

Sediment particles are not allowed to settle on the seabed in areas where the sediment thickness reaches this maximum predefined value. Note that the sediment transport model assumes no feedback from the sediment processes to the hydrodynamic model, and any changes in sediment thickness do not translate into the corresponding changes of the water depth. An 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.

6.13 Wave input

Wave input is represented by the amplitude of the near-bottom wave orbital velocity (m s-1), wave period (s) and wave direction (degrees). The direction angle is given in degrees Cartesian measured from West-East direction counter-clockwise (e.g. North is 90°). Waves are invoked by the key

DO_WAVES YES

The wave data are updated at time intervals given by:

WAVE_VARS_INPUT_DT 1 hour

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

WAVE_VARS waves.nc(direction=wave_dir)(period=wave_per)(ub=wave_ub)

To interpolate waves on the model grid

WAVE_VARS_INTERP_TYPE nn_non_sibson

File "waves.nc" must either include variables named "direction", "period", and "ub" or specify aliases to these names. An alternative to specifying orbital velocity ("ub") is to specify an amplitude of the surface wave, named "amplitude" (the near-bottom velocity in this case is calculated from the linear wave theory).

The default option is no waves.

6.14 Spatial parameters

Spatially varying parameters can be defined by assigning the name of the parameter to the name of a 2d tracer which must be added to the list of tracers. The model will either assign a spatially-uniform distribution to this tracer or it will read it from the netcdf file used to initialise the model. For example:

TRACER30.name PHYSRIPH TRACER30.long_name spatially varying ripple height TRACER30.units m TRACER30.type BENTHIC TRACER30.fill_value 0.01 TRACER30.valid range 0 1 TRACER30.diagn 0

TRACER31.name TRACER5.svel TRACER31.long_name settling velocity of mud TRACER31.units m/s TRACER31.type BENTHIC TRACER31.fill_value -0.01 TRACER31.valid range -1 0 TRACER31.diagn 0

Another approach to define spatially varying parameters can be found in the usermanual of SHOC (hydrodynamic model). One of the options offered is to point TRACER#.svel to the name of a 2d tracer comprising spatial distribution of the velocity:

TRACER5.svel svelOfMud

TRACER31.name svelOfMud TRACER31.long_name settling velocity of mud TRACER31.units m/s TRACER31.type BENTHIC TRACER31.fill_value -0.01 TRACER31.valid range -1 0 TRACER31.diagn 0

6.15 Scaling of Resuspension Rate

With this parameter the user can change the rate of the sediment resuspension. Note that both diffusion flux and resuspension flux contribute to the sediment exchange across water and sediments. The ERFLUX_SCALE changes only the resuspension rate.

ERFLUX_SCALE 0.5

Default value is 1 (i.e. no scaling).

6.16 Example

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

VERBOSE_SED 0

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 $CS\overline{S}0$ 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 0.03 PHYSRIPH 0.6 PHYSRIPL 0.005 BIORIPH BIORIPL 0.2 # Maximum depth for biological activity (m) MAXBIODEPTH 0.2 # Functional form for bioirrigarion 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
                1.0e-9
BI DISSOL KZ I
# 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
WAVE VARS INPUT DT 2 hour
WAVE VARS gbr waves 0 rj.mnc(amplitude=wave amp)(direction=wave dir)
(period=wave per)
WAVE VARS INTERP TYPE nn non sibson
```

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, 2016). This chapter describes tracer parameters specific to sediments.

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 occupy a certain volume in space (inferred from concentration of particles and density of individual grains). They 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 a zero-volume tracer is a sediment-attached tracer (pollutant). Analogous to conventional particles the sediment-attached tracers undergo settling and resuspension/deposition in water column and bioturbation/consolidation in sediments, unlike conventional particles they do not change porosity of sediment layers.



Fig. 7.1 MECOSED tracers

Every MECOSED tracer must be specified as either particulate tracer or dissolved tracer

TRACER4.partic 1

TRACER5.dissol 1

The volumetric tracer is specified using the "calcvol" key:

TRACER4.calcvol 1

Default value for "calcvol" is zero and the traces is considered as having zero volume. If the flag "calcvol" is set to 1 (volumetric tracer) then this tracer is not allowed to attach to any sediment fraction (the key "adsorb" is automatically set to 0).

Comments:

For computational reasons it is recommended to treat biogeochemical reaction variables as zero volume tracers, so that any transient instabilities in the biogeochemical model do not blow away the sediment layer.

!!! Names of volumetric tracers currently are hardwired inside the source-code to a predefined set of sediment classes: Gravel, Sand, Mud, FineSed, Dust, and MetalP. To extend this set, new names must be added to the array SEDCLASS (sediments.c file), and the updated code must be recompiled.

7.2 Initial concentrations

Initial concentration of each sediment fraction is specified individually for each tracer in a tracer description filed. 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 a valid range of the concentration in water and in sediments

TRACER#.valid_range 0 1000 TRACER#.valid_range_sed 0 3000

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

TRACER#.fill_value 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.

Comments:

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). The concentration of a sediment-attached pollutant 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 initial porosity of sediments exceeds 0 but is lower than 1.

Benthic layer of MECOSED must always include sediment particles. In applications with a high-energy environment it is recommended to include in the model a sediment class representing heavy particles (e.g. Gravel) that would form a baseline un-erodible substrate underlying fine sediments.

EMS typically does not resolve bed-load transport. 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 a particulate tracer is given by

TRACER4.svel -0.001

Default is 0.

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

7.4 Cohesive sediment

MECOSED employs different formulations for resuspension of cohesive and noncohesive sediments. A particular sediment resuspension regime is triggered by assigning 0 (non cohesive) or 1 (cohesive) value to the "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.resuspend1TRACER4.deposit1

Default is resuspend and deposit. If both "resuspend" and "deposit" flags are set to 0, then sediment particles neither resuspension nor deposit on the sediment bed. Note that to have benthic and pelagic layers fully decoupled from each other, apart from the resuspension/deposition fluxes, diffusive exchange across water-sediment interface must be switched off too (see section on 6.10 on Biodiffusion),.

7.6 Sediment grain density

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

TRACER4.b_dense 2.65e+03

Note that the sediment grain density and the mass concentration of sediments define 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 along with the sediment grain density defines 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 Mud
TRACER4.long name Mud 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 MECOSED can be attached to any other particulate (partic 1) volumetric (calcvol 1) tracer by setting "adsorb" flag to 1

TRACER4.adsorb 1

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

TRACER4.carriername FineSed

The above strings indicate that the TRACER4 is attached (adsorbed) to the tracer called "FineSed". The tracer "FineSed" must represent some particulate volumetric tracer.

To simulate sorption/desorption exchange between particulate and dissolved fractions of the sediment reactive tracer, the user must 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 MetalD

The above strings indicate that the sediment reactive TRACER4, attached to the sediment tracer "FineSed", has the dissolved counterpart "MetalD".

An equilibrium distribution constant for the desorbed and adsorbed fractions of the sediment reactive tracer is specified by the parameter "adsorbkd" (in m^3/kg)

TRACER4.adsorbkd 20

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

TRACER4.adsorbrate 1

MECOSED 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, MECOSED science manual). Note that concentrations of the sediment reactive tracers are given as an activity per unit volume, rather then 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. TRACER4.name MetalP TRACER4.long name Zn on Fine Sediment TRACER4.type WATER SEDIMENT TRACER4.units g m-3 TRACER4.valid range 0 1e+35 TRACER4.valid_range_sed 0 1e+35 TRACER4.diagn 0 TRACER4.fill value 0.0 TRACER4.fill value sed 0.0 TRACER4.dissol 0 TRACER4.partic 1 TRACER4.advect 1 TRACER4.diffuse 1 TRACER4.b dens 2.65e+03 TRACER4.i conc 1.2e+03 TRACER4.decay 0 TRACER4.adsorb 1 TRACER4.carriername FineSed TRACER4.dissolvedname MetalD TRACER4.adsorbkd 20 TRACER4.adsorbrate 1

Comments:

!!! As of today (June 2018) only one sediment reactive tracer called "MetalP" (particulate) can be simulated without interfering with the source code. To simulate more than one sediment-reactive tracers, the corresponding name (e.g. MetalP2) must be added to the array SEDCLASS (sediments.c file), and the updated code must be recompiled.

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;

A particular 3D 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:

"ustrcw_skin"	bottom shear stress velocity (m s-1)
"depth_sedi"	sediment thickness (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.valid_range_sed 0 1e+35 TRACER7.fill_value_wc 0.0 TRACER7.fill_value_sed 0.0 TRACER7.diffuse 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 netcdf (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, the corresponding data-files must be referenced in the parameter file. For more details on open boundary specifications for simulated tracers please refer to SHOC manual (Herzfeld and Waring, 2016)

8.1 Example of a boundary condition

This section provides an example of boundary conditions for hydrodynamic and sediment variables at the river boundary. Features relevant to the sediment model are highlighted in bold. According to this specification, no-gradient (free-flow) boundary condition is applied to all tracers except FineSed and Dust. The boundary concentrations for FineSed and Dust are defined through the data-file "river_sedi.ts".

```
BOUNDARY 50.NAME
                         Fitzrov
BOUNDARY50.BCOND ELE
                        NOTHIN
BOUNDARY 50.BCOND NOR
                        NOTHIN
BOUNDARY 50.BCOND TAN
                        NOTHIN
BOUNDARY50.BCOND TRA ALL NOGRAD
BOUNDARY50.BCOND FineSed TRCONF
BOUNDARY50.BCOND Dust
                         TRCONF
BOUNDARY50.DATA forcing/fitzroy.ts forcing/river_sedi.ts
BOUNDARY 50. TYPE
                       112
BOUNDARY50.POINTS
                         1
437 55
```

An example of the river boundary data-file ("river_sedi.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 FineSed
## COLUMN2.long_name Fine sediment from catchments
## COLUMN2.units kg s-1
## COLUMN2.missing value -999
```

```
## COLUMN2.fill_value 35
##
## COLUMN3.name Dust
## COLUMN3.long_name Dust
## COLUMN3.units kg s-1
## COLUMN3.missing_value -999
## COLUMN3.fill_value 35
##
-1e13 0.0 0.01
1e13 0.0 0.01
```

9 SHIPS

Mixing of sediments enhanced by ships passing through the study region can be simulated via increased vertical diffusion of dissolved and particular tracers. This enhanced mixing applies throughout the water depth and across the whole cell at the location of the ship. Because of the large uncertainty often characteristic of such studies the problem is handled statistically. The user must specify the typical number of ships passing through the region daily (ship_N), the path they take (i.e. i, j coordinates of grid-cells comprising that path) and a typical time required for a ship to traverse the track (ship_T). The probability for a ship to be found in a particular grid-cell along the track is calculated as

 $P = (ship_T * ship_N) / (24 * ship_C)$

Here ship_C is the total number of the grid-cells comprising the track, and ship_T is given in hours. Once the ship is located in a particular cell, the corresponding vertical diffusion coefficient in set to ship_Kz value (in m^2/s) and all tracers (except temperature and salinity) are mixed vertically.

Ship-parameters are specified in a separate parameter file which is identified by the key SHIP_FILE in the EMS parameter file. For example,

SHIP_FILE pss/shipfile.txt

The "shipfile.txt" must have 5 strings in the header, and 5 numbers in the second line followed by 2 columns of i,j coordinates of grid-cells representing a ship track. The numbers on the second line represent the number of cells on the track, the number of cells on the track (repeated), the number of ships per day, time to travel, and the value of the enhanced diffusion coefficient. An example of the content of the "shipfile.txt" follows

 Ship_cell_i Ship_cell_j Ship_Number Ship_Time Ship_Kz

 4
 4
 3
 2.0
 0.1

 66
 77

 67
 77

 68
 77

 68
 78

10 FILE INVENTORY

The sediment model file inventory is shown in table 9.1.

Ν	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	Trvdiffsettl.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

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