OMEX Biogeochemical Models

The FORTRAN source code of two benthic biogeochemical models developed during OMEX I by the Netherlands Institute of Ecology (NIOO) and a water column biogeochemical model developed by the School of Ocean Sciences, University of Wales (Bangor) are presented on the CD-ROM, together with instructions for their use.

The models included are:

NIOO Models: Sediment Mixing Model

The mixing model was primarily designed to model ^{210}Pb concentration profiles along cores but may be adapted for use with any tracer providing the decay rate is known.

OMEX Diagenesis Model (OMEXDIA)

OMEXDIA is a model of early diagenetic processes including oxic mineralisation, denitrification, anoxic mineralisation and advective-dispersive transport. Its primary result is the modelling of sediment pore water chemistry profiles.

Bangor Model: Microbiological Model (SEDBIOL)

SEDBIOL is a one-dimensional depth-resolving model that couples physical, microbiological and sedimentation plus resuspension sub-models. Its primary result is the modelling of water column profiles.

NIOO Mixing Model

Introduction

The files for the NIOO mixing model may be found in the CD-ROM directory BGMODEL/NIOO/MIXING. This contains the following files:

README.TXT	ASCII notes on using the programs. The following text was based on the information from this file.
MIXING.FOR	Source code for ^{210}Pb concentration profiles.
XSMIXING.FOR	Source code for excess activity profiles.
STATION1.PB	Example input file.
STATION2.CHL	Example input file.
STATIONS.LST	Example program control file.

The remainder of this documentation segment explains how to work with the program "MIXING" or "XSMIXING". MIXING was created by Karline Soetaert (NIOO-Yerseke, the Netherlands, Soetaert@cemo.nioo.knaw.nl) and tests the importance of diffusive mixing/non-local exchange based on measured activity-depth profiles.

The procedures used are explained in

Soetaert, Herman, Middelburg, Heip, de Stigter, van Weering, Epping and Helder. Modelling ^{210}Pb-derived mixing activity in ocean margin sediments: diffusive versus non-local mixing. ***Journ. Mar. Res***., 54: 1207-1227.

Originally the models were created for use with ^{210}Pb profiles; they can also be used with other tracers/substances, provided the decay rate is known.

In the program MIXING, the input is total activity or total concentration; the background production is estimated as an extra parameter. In the program XSMIXING, the input is the excess activity (the background production is not estimated).

Six different models (termed Model1, Model2, Model3, Model4a, Model4b and Model5) are applied on each run.

Model Input

The model requires for each profile that has to be modelled a separate file with observed data. Observed activity or concentrations must be expressed per cm^3, e.g. in dpm/cm^3 or g/cm^3.

This file must have a fixed format. Two examples are enclosed (STATION1.PB and STATION2.CHL).

The format is:

First and second line:	plain text
Third line:	sedimentation rate, e.g. in cm/year
Fourth line:	decay rate, e.g. in per year
Fifth line:	observed profile, in four columns: (column 1) sediment interval from (column 2) sediment interval to (column 3) sediment interval middle (column 4) measured activity in dpm/cm^3 or measured concentration per cm^3

Units may be per day or whatever, but must be consistent. The output then has the same units. For ^{210}Pb we had good results if units were expressed in years; for chlorophyll, units are better expressed in days.

Example file STATION1.PB (^{210}Pb profile; units are expressed per year)

```
Example Pb210 profile to be used with MIXING
from    to      cm  dpm
0.00133
0.03108
0   1   0.5    5.344542
1   2   1.5    4.526892
2   3   2.5    4.319652
3   4   3.5    4.052592
4   5   4.5    5.509152
7   8   7.5    4.221672
9   10  9.5    2.748372
14  15  14.5   1.423908
19  20  19.5   1.464564
```

0.00133 is the sedimentation rate (cm/year) and 0.03108 is the decay rate (per year) of ^{210}Pb. The other lines contain: sediment interval (from, to, mean) and ^{210}Pb activity. For example, line 5 contains data from the 0 to 1 cm horizon which has a mean depth of and an activity = 5.344542 dpm.

Example file STATION2.CHL (chlorophyll concentrations; units are per day)

```
Example chlorophyll ug chl a/ cm3 bulk sediment
from   to   Mean    Conc
0.00001
0.05
0     0.5   0.25    12.7
0.5     1   0.75    6.6
1     1.5   1.25    7.5
1.5     2   1.75    1
2       3   2.5     0.5
3       4   3.5     0.4
4       5   4.5     0.3
5       6   5.5     0.2
6       7   6.5     0.1
7       8   7.5     0.1
8       9   8.5     0.1
9      10   9.5     0.2
10     11   10.5    0.2
```

0.00001 is the sedimentation rate (cm/day) and 0.05 is the first-order decay rate (per day).

The program can test several profiles in one run. Input of the various file names containing the observed data occurs either manually or through a driver file called "STATIONS.LST". This contains a list of the file names to be processed. For example, if the files 'STATION1.OBS' and 'STATION2.OBS' contain the two observed profiles to be tested, then the file STATIONS.LST should look like:

```
STATION1.OBS
STATION2.OBS
```

Model Output

The model generates several output files:

Files 'Model1', 'Model2', 'Model3', 'Model4a', 'Model4b' and 'Model5'

These contain the residual sum of squares, the degrees of freedom and the 'best' parameter values of all the stations fitted with Model 1, 2, 3, 4a, 4b and 5.

File 'LONG'

Contains the output from all models for all stations, i.e. the observed data compared with model-generated activities or concentrations averaged over the sampling interval. Profiles are generated for each model over the first 20 cm and the program reports which model produces the significantly best fit.

File 'ALLMODEL.OUT'

Contains the sum of squared residuals for each model, the number of data and the total sum of squares for each modelled profile.

File 'ALLMODELS.TST'

Contains the result of the F-test statistics for each modelled profile.

The Program

The program was written in FORTRAN.

Maximal dimensions are:

Number of data per station (NMAX):	50
Number of stations or profiles:	30

These are set by a PARAMETER statement.

For each model a number of iterations is performed. The more parameters, the more the number of iterations that are necessary. Also, the more observed data, the greater the number of iterations required.

Currently, the number of iterations are set to:

10	Model1
20	Model2
200	Model3
300	Model4a
300	Model4b
500	Model5

but this may be too large or too low.

The number of iterations are set by a DATA statement.

Because the original data set had too low a resolution below 10 cm and in order to discriminate non-local mixing from diffusive mixing, the depth of the injection site (L) was restricted to [0.5-10 cm]. Also, to avoid overflow, the

minimal bioturbation coefficient is set to 0.0001, the maximal ingestion rate is set to10000 (/year) and the minimal thickness of the ingestion layer is set to 0.001 cm. Depending on the compiler used, these restrictions may not be necessary. All these restrictions are imposed in the subroutine FILLPAR.

Some of the non-local exchange models do not like missing data points and can produce strange results (e.g. giant peaks) if there are missing values.

NIOO OMEX Diagenesis Model (OMEXDIA)

Introduction

The OMEXDIA model was developed by:

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OMEXDIA is a model of early diagenetic processes including oxic mineralisation, denitrification, anoxic mineralisation and advective-dispersive transport.

The model is described in the following papers:

Karline Soetaert, Peter M.J. Herman, Jack J. Middelburg (1996). A model of early diagenetic processes from the shelf to abyssal depths. ***Geochim. Cosmochim. Acta*** 60, 1019-1040

Karline Soetaert, Peter M.J. Herman, Jack J. Middelburg (1996). Dynamic response of deep-sea sediments to seasonal variations: a model. ***Limnol. Oceanogr.*** 41(8), 1651-1668.

Jack J. Middelburg, Karline Soetaert, Peter M.J. Herman and Carlo H.R. Heip. Denitrification in marine sediments: a model study***. Global Biogeochemical Cycles*** 10(4), 661-673.

The essence of the model (compared to more complete diagenetic models) is the lumping of the anoxic processes (using Fe- and Mn oxides and sulphate) into one process which creates a reduced substance, so-called 'oxygen demand units' (ODU). These ODUs are expressed in moles of oxygen needed to re-oxidise them.

The model was originally developed in the simulation environment SENECA, which explains the structure of the code, using common blocks which are generated based on user-defined input files. A lot of the flexibility of the simulation environment is lost though. The model may appear very complex, (and it is) but it is also flexible, facilitating model development.

For those who do not like complex code, the essential model files are source codes NUTRIENT.FOR, CARBON.FOR and TRANSP.FOR (define the

derivates), XSTART.FOR (contains the steady-state solver) and the input files INPUT.PAR and INPUT.VAR (parameter and variable declarations).

The model has been slightly changed since it was described in the first two of the papers cited above:

- The steady-state system is now solved at once, instead of solving C first followed by solving the system for the dissolved constituents. This is because a new way of solving the equations has been implemented; it is now actually faster to solve the entire system in one go.

- The compartmentalisation is somewhat different. In the original model, sediment slices were 0.1 cm thick at the interface, then 0.2 cm and finally were 0.4 cm thick (i.e. [0-0,1], [0.1-0.2], [0.2-0.4], [0.4-0.8] ..). Now the thickness increases exponentially. The interface thickness is set with parameter DXINT (say 0.1 cm). The other sediment slices are a factor SEDLAMBDA thicker than the overlying one i.e. [0-DXINT], [DXINT-DXINT*SEDLAMBDA] etc. (SEDLAMBDA must be larger than 1!).

Files Included on the CD-ROM

The code and data files for the OMEXDIA model may be found in the directory BGMODEL\NIOO\OMEXDIA. The following files are included:

README.TXT	A flat ASCII documentation file on which this documentation was based.
OMEXDIA.FOR	Model source code.
XSTART.FOR	Model source code
CARBON.FOR	Model source code
NUTRIENT.FOR	Model source code
TRANSP.FOR	Model source code
GOODIES.FOR	Model source code
LMODULE.FOR	Model source code
WRCOMMON.FOR	Utility source code (builds common blocks)
XCOMMON.ALL	Common block declarations
XCOMMON.PRG	Common block declarations
XCOMMON.BLK	Common block declarations
XCOMMON.DCS	Common block declarations
OMEXDIA.MAK	Microsoft Developer Studio NMAKE file
INPUT.PAR	ASCII Input file
INPUT.VAR	ASCII Input file
INPUT.RUN	ASCII Input file
INPUT.CAL	ASCII Input file
INPUT.RND	ASCII Input file
INPUT.SEN	ASCII Input file
DYNAMIC.B93	Example observed data file
STEADY.B93	Example observed data file

STEADYO2.B93	Example observed data file
OMEXB93	Example output file
OMEXB93.SUM	Example output file
OMEXB93.S3	Example output file
OMEXB93.CLB	Example output file
OMEXB93.SNS	Example output file
OMEXB93B.SNS	Example output file

Run Modes

There are three different run modes in the model.

- Ordinary run
- Calibration
- Sensitivity analysis

The type of run is set with parameter XSIMRUN (number of simulation runs) in file INPUT.RUN

- When XSIMRUN = 1, an ordinary run is performed.
- When XSIMRUN = X > 1, a sensitivity analysis is performed consisting of X runs. Variables and parameter ranges used in the sensitivity analysis are defined in the file INPUT.SEN.
- When XSIMRUN = X < 0, a calibration analysis is performed with -X runs (40 is the minimal number of calibration runs). Parameter ranges used in the calibration analysis are defined in the file INPUT.CAL.
- When XSIMRUN = 0, a sensitivity analysis is performed based on a predefined input file with parameter values called INPUT.RND. Variables used for the sensitivity analysis are defined in the file INPUT.SEN. The input file INPUT.RND may be easily created from the output generated during calibration by copying and pasting.

All these modes can be applied to either a steady-state or a dynamic simulation.

Source Code

The source code is in seven files:

OMEXDIA.FOR Contains the main program. Calls the other subroutines.

XSTART.FOR	Initialises the benthic sub-model (i.e. steady-state calculation). It is called once at the beginning of the simulation.
NUTRIENT.FOR	Sediment nutrient sub-model. It is called at each time step and is also called for the steady-state calculation.
CARBON.FOR	Sediment carbon sub-model. It is called at each time step and is also called for steady-state calculation.
TRANSP.FOR	Contains the transport sub-module. It is called at each time step by subroutines CARBON and NUTRIENT.
GOODIES.FOR	General program utilities. Reads the settings for the run (run type, simulation time, time step..). Reads parameter values and variable names. Performs the dynamic simulation, integration and output. Performs calibration and sensitivity.
LMODULE.FOR	Linpack utilities used to solve banded systems of linear equations.

There is in addition a utility called WRCOMMON.FOR that generates include files with common block declarations.

User Input

The user-defined input is in ASCII files. They have a fixed structure, described in the file headings.

INPUT.PAR	Contains the parameter values, names, units and descriptions. This file is used to generate common blocks using the program WRCOMMON). Parameter values are read in at the start of the program.
INPUT.VAR	Contains the number of physical compartments (sediment slices) and the number of different substances that are dynamically modelled (state variables). Contains the variable and state variable names, units and description (does NOT contain the names of the rate of change (time derivates) of state variables as these are automatically generated by the utility program WRCOMMON). Defines which variables have to be written to the output files. This file is used by the program WRCOMMON to generate common blocks. Variable names are read in at the start of the program.
INPUT.RUN	Determines the type of run, which may be either a normal run, a sensitivity run or a calibration run. Contains the base name of the output file, the duration of the simulation period (0 if only steady-state run), the time step to be used, the period over which output is averaged and written out, the name of a file containing start conditions (not

used), the names of files containing forcing functions (not used), the name of file containing observed data (used) and the integration routine to be used (Euler or 4th order Runge-Kutta).

If the type of run is not a 'normal' run, other input files are required as well:

INPUT.CAL — Used when the run type is a calibration. Contains the parameter range and the name of the parameters to be used in the calibration.

INPUT.SEN — Used when the run type is a sensitivity analysis. Contains the parameter range and the name of the parameters to be used in the sensitivity analysis. Contains the name of the variables used in the sensitivity analysis.

INPUT.RND — Used when the run type is a sensitivity analysis, with input file of parameter values. Contains the parameter names and values used in the sensitivity analysis. Can be easily made by copying and pasting based on output generated by calibration.

The user has to create new common blocks (using the utility WRCOMMON) and recompile the model when:

- the sequence of parameter names was changed (in INPUT.PAR)
- the sequence of variable names was changed (in INPUT.VAR)
- a parameter was added or removed (in INPUT.PAR)
- a variable was added or removed (in INPUT.VAR)
- more or fewer variables have to be written to output files (INPUT.VAR)
- the number of compartments was changed (XBEN, declared in INPUT.VAR).

It is not necessary to create new common blocks and recompile the model when:

- changing the value of a parameter (in INPUT.PAR)
- changing a run parameter (in file INPUT.RUN)
- changing the description of a variable or parameter

Parameters Used As Switches

Some of the parameters defined in file INPUT.PAR need some extra explanation. They define the numerical approximation of the model.

SEDLAMBDA — Defines the degree of increase of the sediment thickness. When set to 1, all sediment layers are equally thick. When set to 1.1, layer 2 is 1.1 times as thick as layer 1 and so on. It can be used, together with the number of slices (or model compartments XBEN, defined in INPUT.VAR) and the interface thickness (DXINT) to determine the total sediment thickness that is modelled. The factor cannot be set too high because of increased numerical dispersion (especially when using the Fiadeiro & Veronis numerical scheme).

DXINT — The thickness of the interfacial layer, in cm.

FIADEIRO — Determines whether the numerical scheme of solid substances uses centred differences (when set to 0) or the differences according to Fiadeiro & Veronis (1977)- ***Tellus*** 29, 512-522. The latter switches gently from centred to backward differences as the importance of advection compared to bioturbation increases. It is an unconditionally stable scheme but it can lead to large numerical dispersion when the sediment slices in the zone of predominant advection are too large. (Personally we prefer centred differences, but these can be problematic when concentrations of solid substances increase with depth into the sediment e.g. when including non-local exchange phenomena).

Observed Data

Observed data files are used to estimate the goodness of fit of the modelled output versus measurements. The goodness of fit is calculated in file GOODIES.FOR.

There are two types of observed data (and two types of goodness of fit):

- In the case where the run is dynamic (parameter NTIME in 'INPUT.RUN' >0), the observed data must consist of measurements versus time. An example is in file 'DYNAMIC.B93', containing fictitious oxygen and nitrate fluxes on various sampling days.

- In the case where the run is a steady-state calculation (parameter NTIME in 'INPUT.RUN' = 0), the observed data consist of sediment depth profiles. Examples are in file 'Steady.b93' or 'SteadyO2.b93'.

The goodness of fit of model/observations is calculated as the sum of the absolute values of residuals of modelled versus observed values, standardised for the standard deviation of the observations. There is a goodness of fit for each observed variable and a model goodness of fit (= sum of variable GOFs). The model goodness of fit is used in the calibration procedure.

Common Blocks - Include Files

The model uses common blocks to pass the values of variables, state variables and parameters among subroutines. They are defined in the include file 'XCOMMON.BLK'. These common blocks are generated by a utility program called WRCOMMON. It uses the ASCII files INPUT.PAR and INPUT.VAR to generate the common blocks.

For each state variable (SVAR), a new variable containing the rate of change, with name DSVAR is created. For example, if a state variable NH3 has been defined in INPUT.VAR, with 100 physical compartments (XBEN = 100), then the program WRCOMMON generates room for two arrays called NH3(100) and DNH3(100), where the latter contains the rate of change.

After generating new common blocks, the entire model has to be recompiled.

The program WRCOMMON creates common blocks in an include file called 'XCOMMON.BLK.' and constants defining the model in an include file called 'XCOMMON.DCS'.

The include file 'XCOMMON.BLK' contains:

- a common block with parameter names, called XCBPAR
- a common block with state variable names and their derivates, XCBSVAR
- a common block with the ordinary variables called XCBVAR

The include file 'XCOMMON.DCS' contains:

- the number of physical compartments in the model. They are XBEN, the number of benthic compartments (sediment slices), XVER, the number of vertical pelagic compartments (not used in this model) and XLAT, XHOR, the number of horizontal pelagic compartments (not used in this model).
- the number of nutrients in the model (different state variables) (XNUT)

- the total number of state variables (XMXSVAR)
- the total number of ordinary variables (XMXVAR)
- the number of parameters (XMXPAR)
- the number of output variables (XNOUT)

The include file 'XCOMMON.ALL' contains variables and parameters which are common to the diagenetic sub-model (e.g. bioturbation profiles, porosity profiles,..). This file as not affected by the program WRCOMMON.

The include file 'XCOMMON.PRG' contains declarations of variables and parameters used for general program flow (e.g. the time step, starting time, file names etc..).

Model Output

The model generates various ASCII output files. The base name of output files is defined in the file 'INPUT.RUN'. If for example this base name is 'OMEXB93' then the model will generate the following output files:

During an 'ordinary run':

OMEXB93 Contains the parameter values (to recognise the run) and the steady-state characteristics of the current run.

OMEXB93.SUM Contains summary statistics of output variables during a dynamic run: minimal value, maximal value, mean value and the goodness of fit with observed data.

During a 'dynamic run'

OMEXB93.S1-6 Six files generated containing output of state variables, at certain time intervals. There is one file for each state variable containing data for all compartments. For example, if FDET is the first state variable declared in file 'INPUT.VAR' and there are 50 compartments (XBEN = 50 in 'INPUT.VAR'), then the file OMEXB93.S1 will contain values of FDET(1) ..FDET(50) as they change in time.

OMEXB93.V1-2 Two files generated containing output of ordinary variables, at certain time intervals. There are 'XBEN' ordinary variables per output file (XBEN = the number of sediment slices). For example, if TOC is the first ordinary

variable, defined in 50 compartments, the file OMEXB93.V1 will contain values of TOC(1) .. TOC(50).

Whether or not the variables have to be written to the output may be controlled by defining them above or below the '{' mark in the file INPUT.VAR (don't forget to make new common blocks if variables are moved above/below the '{').

The model generates output which is averaged over a certain period, the length of which is defined in the file 'INPUT.RUN'.

Output generated during a 'calibration run' may be found in file OMEXB93.CLB, containing the initial and ultimate parameter ranges and values.

Output generated during a 'sensitivity run' may be found in file OMEXB93.SNS, containing parameter values and goodness of fit and total range of output variables.

Integration

With each array of state variables, an array containing the rate of change is declared in the common block. For example, if a dynamically modelled substance, defined in 50 compartments (XBEN=50), is called NH3, there is a declaration NH3(50) and DNH3(50) in the common block XCBSVAR.

Before calling the user-supplied subroutines (i.e. nutrient, carbon) the rates of changes of all state variables are set to 0 (in subroutine DYNARUN, file GOODIES.FOR).

These rates of changes can then be changed in subroutines nutrient or carbon like this:

```
DNH3(I) = DNH3(I) + INPUT - OUTPUT
DNH3(I) = DNH3(I) - NITRIFICATION
etc..
```

Integration need not to be done in the user-supplied subroutines. It is performed in the subroutine DYNARUN (in file GOODIES.FOR).

The model uses either plain Euler or 4^{th} order Runge-Kutta to integrate. It uses a fixed time step, as defined in the input file 'INPUT.RUN'. In practice the time step should be small enough to avoid instabilities (how small depends on how fast forcing functions change in time, on the thickness of sediment slices ...).

The use of 'stiff' integrators like Vode is not supported in this version, but they can easily be added to subroutine DYNARUN, although some rearranging of the way the state variables and their derivates are supplied to VODE is required, in a way similar to subroutine MNEWT, in file XSTART.FOR).

Compilation

If changes are made to the input files INPUT.PAR and/or INPUT.VAR, the utility program WRCOMMON should be run, in order to create the include files with common blocks used in the model.

The model may then be compiled.

The model was originally implemented in the 'Microsoft FORTRAN 77' compiler and then migrated into the 'Microsoft Developer studio' (FORTRAN Power Station Version 4.0).

To work efficiently, both the source code and the input files were included in the project (to make sure that changes in the input files are saved before starting a new run).

Model Development

The model structure is complex, but it is easy to change the formulations.

- Changing the number of physical compartments

  Change the value of XBEN in file INPUT.VAR.

  Run the utility WRCOMMON (to generate the common blocks).

  Recompile the model.

- Adding new state variables

  Change the value of XNUT in file INPUT.VAR and add the new name(s) (the first XNUT lines after the declaration of XNUT contain the names of the state variables). Do not define the name of the corresponding rate of change.

  Run WRCOMMON; now the new state variables are known to the other subroutines.

  Add new descriptions in the FORTRAN source files.

  Recompile the model.

- Adding new (ordinary) variables

  If the variables have to be written to an output file, declare them in INPUT.VAR, above the line beginning with the '{' mark.

  Run WRCOMMON and recompile.

  If the variables do not need to be written to an output file, declare them in INPUT.VAR, below the line beginning with '{'.

  Recompile.

  If the variables have to be known only locally, they can be declared in the source code.

- Changing the model formulations

  The model has been structured such that new formulations may be added easily. The Steady-state solver is (almost) independent of the formulations used. It requires however that transport can be written in tridiagonal form, i.e. translocation between distant layers is not supported (but non-local exchange, where sediment is taken from the surface and injected into the sediment is possible).

Example Output Files

Seven example output files are included.

- An ordinary dynamic run (XSIMRUN = 1 in file 'INPUT.RUN') was performed:

  For 365 days (NTIME = 365 in 'INPUT.RUN').

  Using a time step of 0.00048828125 days (TIMEST in file 'INPUT.RUN' = 0.0004; the integration routine then searches for the nearest exact multiple of 2, to avoid rounding error).

  Using observed data file 'DYNAMIC.B93' (oFILENAME = DYNAMIC.B93).

  Using Euler integration (XINTTYPE = 1).

  The output interval (and the period over which output is integrated) was set to 1 day (OUTFACT = 1).

  Some of the output files generated were:

OMEXB93 Steady-state characteristics before starting the dynamic run.

OMEXB93.S3 O2 concentration profiles during a dynamic run. (365 days). The depth of each sediment slice may be found in file 'OMEXB93'.

OMEXB93.V2 Fluxes, contribution of oxic mineralisation etc. during the dynamic run.

OMEXB93.SUM Summary output file of the dynamic run.

- 300 sensitivity runs were performed (XSIMRUN = 300) for the steady-state version of the model (NTIME = 0).

  The observed data file was 'STEADY.B93' (oFILENAME).

  The parameters included in the sensitivity analysis were:

  total mineralisation rate (TotMin)
  the part of detritus that is fast decaying (PartFDET)
  and the bioturbation rate (Biotur).

  They are declared, with their ranges in 'INPUT.SEN'.

  The variables that needed to be tested were O2, NO3, NH3, TOC (1st 20 compartments only) and the various fluxes. They are declared in file 'INPUT.SEN'.

  The output file generated was OMEXB93.SNS. It provides for each run the parameter values used (for Totmin, PartFDET, Biotur) and the goodness of fit with O_2, NO_3, NH_3, and TOC profiles as given in the observed data file 'STEADY.B93'. The last column is the model goodness of fit. Finally the minimal, maximal and mean value for each of the sensitivity variables is given.

- 500 calibration runs were performed (XSIMRUN = -500) for the steady-state version of the model (NTIME = 0).

  The observed data file was 'STEADYO2.B93' (oFILENAME). This file only contains an observed oxygen profile.

  The parameters included in the calibration analysis were:

  total mineralization rate (TotMin)
  the part of detritus that is fast decaying (PartFDET)
  the bioturbation rate (Biotur)
  the decay rate of fast (cFDET20) and slow detritus (cSDET20) at 20 dg.

These parameters and their ranges are declared in 'INPUT.CAL'

The output file generated was OMEXB93.CLB. This provides first the initial and ultimate parameter values (for Totmin, PartFDET, Biotur, cFDET20 and cSDET20) and the obtained range in goodness of fit (note that only the range for TotMin has been significantly reduced). Then for the 40 best runs, it gives model goodness of fit (which is equal to the goodness of fit with respect to the O_2 data in STEADYO2.B93) and the parameter values.

- 40 sensitivity runs were performed using parameter values in input file 'input.RND' (XSIMRUN = 0) for the steady-state version of the model (NTIME = 0).

  The observed data file was 'STEADY.B93' (oFILENAME)

  The parameter values included in the sensitivity analysis were obtained by copying and pasting from the output generated during the calibration exercise (from file OMEXB93.CLB pasted into INPUT.RND).

  The variables that needed to be tested were O_2, NO_3, NH_3, TOC (1st 20 compartments only) and the various fluxes. They are declared in file 'INPUT.SEN'.

  The output file generated was OMEXB93B.SNS. It provides for each run the parameter values used and the goodness of fit with O_2, NO_3, NH_3, and TOC profiles as given in the observed data file 'STEADY.B93'. The last column is the model goodness of fit. Finally the minimal, maximal and mean value for each of the sensitivity variables is given.

SEDBIOL Microbiological Model

Introduction

The SEDBIOL model is a 1-dimensional, depth-resolving model that couples physical, microbiological and sedimentation/resuspension sub-models. It was developed to simulate conditions on a shallow (~200 m) shelf station on the Goban Spur.

There are two variants of the model. The first, SB1BOX, includes a single microplankton compartment incorporating phytoplankton, bacteria and protozoa smaller than 200 microns. The second, SB2BOX, has two microplankton compartments. The first of these represents spring microplankton (diatoms and associated protozoa) and the second represents a microplankton dominated by small cells.

The source code for each model variant and initial value files for two definitive documented runs of the SEDBIOL model have been supplied. These are known as 'Run 2' (SB2BOX) and 'Run 7' (SB1BOX).

Run 2 is one of the model runs described in:

Smith, C.L. and Tett, P. (submitted). Parameterisation of a numerical model containing one and two microplankton compartments. Submitted to Journal of Plankton Research.

Run 7 is one of the model runs described in:

Smith, C.L. and Tett, P. (submitted). A depth resolving numerical model of physically forced microbiology. Submitted to Estuarine Coastal and Shelf Science.

Files on the CD-ROM

The model source code and initial value files may be found in the CD-ROM directory BGMODEL\BANGOR. This directory contains two sub-directories, one for each run, called RUN2 and RUN7 containing the following files.

RUN2\SB2BOX.F	FORTRAN source code for the two microplankton compartments model variant.
RUN2\LGSI10.BLM	Initial value file for Run 2.

RUN7\SB1BOX.F	FORTRAN source code for the one microplankton compartment model variant.
RUN7\LGSKZ50.BLM	Initial value file for Run 7.

The FORTRAN source code supplied is internally documented through the liberal use of plain language comments, including a full description of the function of all variables and arrays.

The structure of the input file LGSI10.BLM is as follows:

0.005 30 0.19	Time step, number of depth bins and the maximum permitted value for N_z and K_z (prevents instability whilst keeping time step reasonable).
200.00	Mean depth.
2.5E-3	Bottom quadratic friction coefficient.
367.0	Simulation length in days.
49.5	Latitude for simulation.
0.0001	Background eddy viscosity.
1.1452e-06 1.2595e-06	X and Y components of the tidal velocity.
6.88 8.236	X and Y phase differences.
7.85 1.8 2.59	Mean, amplitude and phase of a sine wave predicting wind speed.
133.55 112.94 -0.38	Mean, amplitude and phase of a sine wave predicting solar radiation.
9.19 3.74 -1.24	Mean, amplitude and phase of a sine wave predicting dew point temperature.
1	Weather control switch (0 = derived from sine wave, 1 = derived from perturbed form of sine wave).
8.0	Initial temperature.
9.0	Initial nitrate concentration.
1.0	Initial ammonium concentration.
0.8	Initial chlorophyll concentration.
3.4	Initial microplankton carbon concentration.
0.2	Initial microplankton nitrogen concentration.
1.0	Initial detritus carbon concentration.
0.1	Initial detritus nitrogen concentration.
300.0	Initial oxygen concentration.