

## **Ecological modelling**

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### **Summary of results obtained in 1998-1999**

Within the OMEX community, our task consists in the testing of ecological formulations for use in the 3-D hydrodynamical models, developed and run by IST and SINTEF. This requires a flexible method to implement and improve models, as well as facilities of data assimilation.

As the bulk of observed data will become available the coming year, we have focussed on the more technical aspects of our models. We mainly increased the facilities to efficiently adapt existing models, make new models and assimilate observed data. This has resulted in a 'modelling environment' in which all routines handling the technical aspects have been automated and can be triggered without any coding.

### **Modelling tools**

#### ***General model structure***

All our models have the same structure and are completely based on ASCII files. As such the models can be entirely managed in a FORTRAN programming environment.

The models that have been developed in OMEX are: the diagenetic models (various versions), the turbulence-closure model, the coupled physical-pelagic-benthic model, the set of phytoplankton models.

Each of these models consists of a model-specific and a general part:

- a set of model-specific FORTRAN subroutines
- ASCII input files (model-specific)
- ASCII (observed and/or forcing function) data files (model-specific)
- a set of files containing general FORTRAN subroutines (the same for all models).

A help page, explaining all the details of the model environment, has been developed.

#### ***Facilities of the models***

The main options available in our models are briefly outlined below. A full account of capabilities can be found in the help page, accompanying the models.

A model option is set by specifying the setting of a keyword in an ASCII input file (called input.run). All the options can be combined at will.

- Run types

Our models may run in various modes, *i.e.*:

- (1) a normal run, *i.e.*, running the model once, producing output and calculating goodness of fit
- (2) a calibration run, *i.e.*, finding parameter values that best fit the observations
- (3) sensitivity runs (2 types), determining the sensitivity of certain output variables to specified parameters
- (4) a Monte Carlo analysis,
- (5) batch runs, performing several model runs consecutively.

- Steady-state calculation

The steady-state condition of a model (where the rate of change is zero) can be calculated in two ways, either (1) by an iterative root-finding routine, an optimised Newton-Raphson method (used in the diagenetic model), or (2) by dynamically running till steady-state is reached (used in the set of phytoplankton models).

Additional options are available, *e.g.*, it is possible to calculate steady-state for a subset of the model equations, it is possible to test for a 'recurrent' steady-state (with a certain periodicity), *etc.*

- Integration routines: We have implemented

- (1) Plain Euler integration, (used *e.g.*, in turbulence-closure and coupled model)
- (2) Euler with adaptive time step,
- (3) 4-th order Runge-Kutta, (used in phytoplankton models)
- (4) 5-th order Runge-Kutta and
- (5) a stiff integration routine (DVIDE, from the linpack routines, used in the diagenetic model)

- Initial conditions: Initial conditions of state and output variables can be specified as:

- (1) one value for each state variable. Used when restarting the model using final conditions from a previous run.
- (2) a depth profile; used for variables with a spatial resolution. In this way, one can change the spatial resolution of the model without the need to specify new start condition files.

- Forcing functions: When declared in a special ASCII file, all forcing functions are automatically updated by the model and can be addressed in the model-specific routines as ordinary variables. They can be specified as:

- (1) a plain data series, or
- (2) a data series consisting of profiles.

- Observed data: Observed data are used to calculate the goodness of fit of the model to the data. This is used in the calibration routines. Observed data can be specified as:

- (1) a plain data series,
- (2) a data series of profiles,
- (3) a set of experimental conditions (used in the phytoplankton models).

- Calibration routines: Four calibration routines are implemented. Two are based on randomised search methods, two are 'greedy' algorithms; each routine can be fine-tuned by means of additional settings (not specified here). The routines are:

- (1) a pseudo-random search algorithm (which can run on several computers at the same time)
- (2) the method of simulated annealing,
- (3) Powells direction-set method
- (4) the Levenberg-Marquardt algorithm.

In addition, there are various possible ways to assess the goodness of fit of observed variables and model, *i.e.*, as the sum of squared residuals, or as the sum of the absolute values of the residuals. The 'model goodness-of-fit' is either a weighted sum of the variable goodness of fit, or as the maximal value of variable goodness-of-fit. Weighing of variable goodness of fit is either *via* the standard deviation or variance in the data, or by user-specified errors.

- Output: Output consists of ASCII files that contain:

1. A time series of state variables and ordinary variables, in spreadsheet format or in database format. (dynamic runs)
2. Stop conditions of the state variables (dynamic runs)
3. Steady-state conditions of the state (and other) variables (steady-state runs)

4. A list of all run settings and parameter values used
5. The summary statistics of all variables. This file contains all the information needed to derive detailed budgets.

The output is visualised by means of EXCEL spreadsheets. These contain a Visual Basic program that facilitates reading of model output and comparing the output from various runs.

- Other facilities: These deal with the details of how the model runs, *i.e.*, how the random number generator is initialised, how random parameter values are created, what is written to the screen, etc.

## **Account of deliverables during 1998-1999**

### ***Workpackage II. PELAGIC***

#### ***Task II.3.3. Turbulent closure in pelagic models***

We added the facility to impose a forcing function as a time series of (vertical) profiles. This will enable us to impose the profile of vertical diffusion coefficients as measured by UWB-b to the 1-D model of the Lagrangian experiment that we will model next year.

UWB-b estimated a lower bound of vertical diffusivity of  $4-13 \cdot 10^{-4} \text{ m}^2 \text{ s}^{-1}$  that will be imposed to our turbulence-closure formulation.

#### ***Task II.4.3. Nutrient boundary fluxes***

Assemble nutrient database: postponed till the last year, until more data are in the BODC database.

#### ***Task II.8.3. Parameterisation of primary production***

Model P *versus* I curves and relate to depth

The more complex phytoplankton model implemented during the first year will be tested to the depth-variation of P *versus* I curves. If these are caused by the variable physiological condition of the algae, this model should be able to reproduce the trends.

### ***Workpackage III. BENTHIC***

#### ***Task III.1.6. Benthic model***

Awaiting the parameterisation and abstraction of the near bed physical processes performed by POL. The 2-D slice model developed by POL, without the near bed physical processes, has been made available (Dr. Xing). It is currently being tested and will possibly be used to embed the pelagic formulations.

#### ***Task III.2.4. Modelling benthic fluxes.***

The benthic diagenetic model has been extended with the Fe, Mn, S cycle, and now includes Si dynamics. This has been done in unity with our involvement of the EU projects EROS-2000 and METROMED.

The calibration routines implemented in our models will facilitate validation and calibration of these models with field results.

#### ***Task III.3.6 Ecological modelling***

The role of the benthic community is included in the diagenetic model as (1) a first-order decay coefficient of organic matter, and (2) a bioturbation coefficient. Both can be estimated based on models developed during OMEX-I; the former *via* the fully coupled diagenetic model, the latter *via* our  $^{210}\text{Pb}$ -decay models.

### ***Workpackage IV. INTEGRATED MODEL***

*Modelling benthic-pelagic coupling.*

Various formulations of benthic-pelagic coupling have been tested during the first year of OMEX II. A manuscript has been written and submitted.

Meta-modelling of the results of the diagenetic model calibrated against field measurements will constitute the basis of the formulations that will be eventually used in the 3-D model.

*Modelling benthic cycling and burial.*

Diagenetic processes can be modelled using the OMEX I diagenetic model, extended during OMEX II-II. A newly added integration routine has increased computational speed for the dynamic mode with several orders of magnitude.

**Outline of work that will be performed in 1999-2000**

During the OMEX meeting in Plymouth (April 99) it was decided, in agreement with the Work Package leaders, that we will first implement a complex ecosystem model, that will be calibrated against the data gathered in the Lagrangian experiment (Workpackage I). Sensitivity and Monte Carlo analysis will then form the basis for reducing the model complexity such that it can be used in the 3-D hydrodynamical model.

Formally we are not involved in Workpackage I. Nevertheless, as it consists of a short-term experiment of limited spatial extent, the resulting ecological model will be fast and more easily tested than when incorporated in a 3-dimensional framework.

Figure: schematic outline of model structure for two models, the turbulence-closure model (left) and the diagenetic model (right).

