

REPORT. No. 20
The Hamburg Oceanic
Carbon Cycle Circulation Model
Version “HAMOCC2s”
for long time integrations

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1 SUMMARY PAGE

The Hamburg Ocean Carbon Cycle Circulation Model (HAMOCC, configuration HAMOCC2s) predicts the atmospheric carbon dioxide partial pressure (as induced by oceanic processes), production rates of biogenic particulate matter, and geochemical tracer distributions in the water column as well as the bioturbated sediment. Besides the carbon cycle this model version includes also the marine silicon cycle (silicic acid in the water column and the sediment pore waters, biological opal production, opal flux through the water column and opal sediment pore water interaction). The model is based on the grid and geometry of the LSG ocean general circulation model (see the corresponding manual, LSG = Large Scale Geostrophic) and uses a velocity field provided by the LSG-model in “frozen” state.

In contrast to the earlier version of the model (see Report No. 5), the present version includes a multi-layer sediment model of the bioturbated sediment zone, allowing for variable tracer inventories within the complete model system.

1.1 MAIN AUTHORS OF THE MODEL

- Ernst Maier-Reimer, Max-Planck-Institut für Meteorologie, Hamburg, Germany
- Christoph Heinze, Max-Planck-Institut für Meteorologie, Hamburg, Germany

2 MODEL DESCRIPTION

2.1 GENERAL APPROACH

The model simulates the inorganic carbon cycle, part of the the organic carbon cycle, and the silicon cycle of the world ocean. Additionally to the ocean water carbon reservoir the atmosphere and the bioturbated sediment (solid components, porewaters) are considered. The water-column-sediment-system is regarded as the interface between input of matter from terrestrial sources and output to the lithosphere. The input rate of terrigenous matter is prescribed. The global output rate through sediment accumulation – as computed by the model – approaches asymptotically the same value, however with a different spatial structure than the input field. In contrast to earlier model configurations (e.g., Maier-Reimer and Bacastow, 1990; Bacastow and Maier-Reimer, 1990; Heinze et al., 1991; Maier-Reimer, 1993) therefore, here, the total inventories of matter in the model are variable. In a complete equilibrium state of the model, however, the inventories stabilize at a constant value.

The model version described here, uses a 1-year time step. Its special purpose are longterm integrations over 10,000s of years, especially reasonably fast model runs to equilibrate the full system including the bioturbated sediment. It is an improved and updated version of the basic configuration used in Heinze et al. (1999). (Model versions including the seasonal cycle are available also, but not described here; please see Maier-Reimer, 1993; Six and Maier-Reimer, 1996; Bareille et al., 1998; Maier-Reimer and Henderson, 1998. The work of Bareille et al., 1998, also includes an interactive multi-layer sediment module.)

The internal oceanic redistribution of tracers within the ocean water is based on the velocity field and the thermohaline fields of the dynamical Hamburg Large Scale Geostrophic Ocean General Circulation Model (LSG OGCM). This dynamical model including sea ice cover is described by Maier-Reimer et al. (1993) as well as Maier-Reimer and Mikolajewicz (1992) (Deutsches Klimarechenzentrum, Technical Report No. 2). For the carbon cycle model, the velocity and thermohaline LSG fields are read from input files and are not computed explicitly. For convective mixing annual integrals of the local convection events are used in the annually averaged carbon cycle model to account for this effect of seasonality in spite of the 1-year time step. The parameterisation is equivalent to a diffusive process, where the diffusion coefficient depends on the duration of hydrostatic instability at the respective grid point per year.

The carbon cycle model’s basic structure is derived from the geochemical concept as described in the work of Broecker and Peng (1982, pp. 2-11), the sediment part of the model closely follows Archer et al. (1993). The “biological matter pump” is simulated with its two carbon components – the organic carbon pump and the calcium carbonate counter pump – as well as the biogenic silica (opal) component. Only phytoplankton export is considered (for a model version taking into account also zooplankton dynamics, please, see Six and Maier-Reimer, 1996). Only the production which is exported (leaves the euphotic zone) is modelled. Besides the soft tissue of organisms (particulate organic carbon, POC), biogenic hard part production of calcareous and opaline material is simulated. POC and opal export production are computed on the basis of available nutrients in the surface layer (in the model, biolimiting nutrients are phosphate and silicic acid respectively). CaCO_3 shell material production is calculated on the basis of the ratio POC-production:opal-

production. By this formulation the marine carbon and silicon cycles are coupled in the model (Heinze et al., 1999). The biogenic particulate matter is redistributed within the water column making assumptions about the redissolution rate and sinking velocity which are both summarized in an exponential particle penetration profile. The organic particulate carbon is remineralised under oxygen consumption. Remineralisation stops if oxygen sinks to a given threshold value. The model carries suspended particulate organic carbon as a tracer. CaCO_3 and opal particles which do not reach the sediment are treated as if they would redissolve immediately. The amount of the particle export production which is not remobilised within the water column plus a fixed rain of chemically inert clay are deposited on the top layer of the bioturbated sediment. The sediment module mimics the chemical pore water solid matter interactions, porewater diffusion, vertical advection of sediment, and bioturbation. The bottom layer of the open water column and the sediment pore waters exchange matter through diffusion. The difference of particle rain minus redissolved matter is finally accumulated in the sediment (leaving the bioturbated sediment zone; see Archer et al., 1993). In order to close the cycle weathering fluxes of matter entering the ocean from the continents are prescribed. The input is performed homogeneously at the surface ocean leaving space for future refinements.

The carbon cycle model includes a simple atmosphere model with only diffusive transport of CO_2 and O_2 and only in meridional directions (assuming perfect zonal mixing). Gas transfer between ocean and atmosphere is carried out with a simple bulk formula.

The model can either be run for the full 3-dimensional case or optionally in reduced 1-dimensional case with fixed fluxes and concentrations in the water column but variable sediment tracers. Also, the model can be integrated with or without rare carbon isotopes ^{13}C and ^{14}C besides ^{12}C .

2.2 TRANSPORT OF TRACERS WITH OCEAN VELOCITY FIELD

All dissolved and suspended water column tracers are transported with the ocean velocity field using the tracer transport equation (continuity equation for amount of matter):

$$\frac{\partial c}{\partial t} = -\text{div}(\vec{v} \cdot c) - q \quad (1)$$

where

- c : tracer concentration
- t : time
- $\vec{v}$: velocity vector
- q : sources and sinks

Details of the numerical advection algorithm are described in more detail in the paragraph on subroutine `advect` below.

Uptake of phosphate and silicic acid as biolimiting nutrients by phytoplankton in the surface layer is the only additional process (sink) included in the tracer transport equation. Uptake of nutrients by organisms is included in this equation to allow for faster uptake rates than 1 per year. All the other chemical interactions and also radioactive decay of ^{14}C (a slow process) are calculated in separate routines (time splitting method).

2.3 BIOLOGICAL PRODUCTION OF PARTICULATE MATTER

Three species of biogenic particles are considered by the model: POC (particulate organic carbon), CaCO_3 (calcium carbonate), and opal (biogenic silica). For POC and opal, biological export production of particulate matter is assumed to follow Michaelis-Menten-kinetics of nutrient uptake (e.g., Parsons and Takahashi, 1973):

$$P_c = \frac{dc_{particulate}}{dt} = c \cdot \frac{V_{max/n} \cdot c}{K_{s/n} + c}; \quad V_{max/Si(OH)_4} > V_{max/PO_4} \quad (2)$$

where

- P_c : production rate of opal or POC respectively
- c : nutrient concentration (silicic acid or dissolved phosphate)
- $V_{max/n}$: maximum uptake velocity of substance n
(n = silicic acid or dissolved phosphate)
- $K_{s/n}$: half saturation constant for substance n

The uptake rate of silicic acid is assumed to be faster than that for phosphate resulting in larger horizontal gradients for opal than for POC production. This leads to production ratios P_{opal}/P_{POC} which are high in eutrophic and low in oligotrophic regions. The export production of CaCO_3 is coupled to the local production ratio P_{opal}/P_{POC} . It starts to increase gradually (parameter R see below) if P_{opal}/P_{POC} sinks below a threshold value S_{opal} :

$$P_{CaCO_3} = P_{POC} \cdot R \cdot \left(1 - \frac{P_{opal}/P_{POC}}{S_{opal}}\right), \quad P_{opal}/P_{POC} < S_{opal}; \quad (3)$$

$$P_{CaCO_3} = 0, \quad P_{opal}/P_{POC} \geq S_{opal} \quad (4)$$

where

- R : maximum possible rain ratio $\text{C}(\text{CaCO}_3):\text{C}(\text{POC})$
- S_{opal} : threshold value of P_{opal}/P_{POC} for
begin of CaCO_3 production

Both, S_{opal} and R , are tunable model parameters.

2.4 SEDIMENTATION

The vertical flux of biogenic particulate matter is parameterised through exponential redistribution profiles which implicitly include both, sinking velocity and redissolution rate. The amount of export production reaching a certain depth level is then given by

$$F(z) = P(z_0) \cdot e^{(z-z_0)/d_p}$$

where

$F(z)$: particle flux at depth z
 $P(z_0)$: export production of particles
 z_0 : depth of interface between surface layer and second layer
 z : depth at which flux is to be calculated
 d_p : depth where flux is $1/e$ of export production

The amount of particles leaving the lowermost wet box of the water column is considered as deposition rate onto the uppermost sediment box.

The model sediment consists of several layers varying in thickness and porosity (amount of pore water volume as part of the total sediment volume). The vertical resolution decreases with depth. Only the “sediment mixed layer” or bioturbated zone is considered (i.e., that part of the sediment column, which is not yet diagenetically consolidated and is mixed through bioturbation by worms and other organisms; compared to common oceanographic language, for the sediment, mixed layer does not mean complete vertical homogeneity as assumed for the ocean mixed layer at the sea surface).

The sediment module follows the concept given by Archer et al. (1993) with the simple expression:

$$accumulation = deposition - redissolution$$

Major processes are redissolution and remineralisation of biogenic particulate matter through reaction with the pore waters, diffusive transport of pore water tracers and diffusive exchange with the bottom waters of the free water column, vertical sediment advection as well as accumulation, and bioturbation. The basic equations for solid sediment components S and concentrations of dissolved substances P within the pore water are:

$$\frac{dS}{dt} = D_B \frac{\partial^2 S}{\partial z^2} - \frac{\partial}{\partial z}(w \cdot S) - \frac{R \cdot M}{\rho \cdot (1 - \Phi)} \quad (5)$$

$$\frac{dP}{dt} = \frac{\partial}{\partial z}(D_W \frac{\partial P}{\partial z}) + \frac{R}{\Phi} \quad (6)$$

where

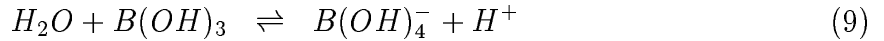
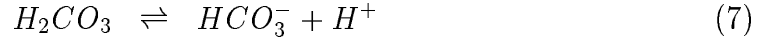
S : solid component (in weight fraction of total sediment)
 P : dissolved pore water component
 D_B : diffusion coefficient for bioturbation
 w : vertical advection velocity of solid compounds
 R : reaction rate
 M : molecular weight of solid component
 ρ : density of bulk sediment
 Φ : porosity
 D_W : diffusion coefficient for pore water diffusion.

Particle deposition, pore water chemistry, and pore water diffusion (processes with short time constants) are carried out simultaneously, while sediment accumulation and bioturbation (processes with long time constants) are computed separately. The simplifying assumption is made, that the specific weight of sedimentary matter is constant regardless

of composition. The vertical advection of solid sediment is computed by requesting a constant geometry of the bioturbated sediment layers and continuity of volume. The burial flux into the “lithosphere” (the sediment accumulation rate) tends to balance the inflow of matter. This input from terrestrial sources (weathering of continental crust) is prescribed as a constant matter flux at the sea surface. When the modelled tracer distributions approach equilibrium during an integration the global integrals of the accumulation rates approach the respective global integrals of the input rates for the respective species of matter. The global values of the accumulation rates therefore are no prognostic variables in the present model configuration. The spatial distribution of the accumulation rates, however, is a prognostic variable and is not prescribed.

2.5 THE INORGANIC CARBON CYCLE

The treatment of the inorganic carbon cycle is conceptually equal to the procedure as described in Maier-Reimer and Hasselmann (1987). A detailed description of marine inorganic carbon chemistry is given by DOE (1994). Besides the two dissociation steps of carbonic acid the borate buffer is considered. For the computation of the CO_2 partial pressure (or the free carbon dioxide in water H_2CO_3) the following reactions have to be considered:



Given the total number of carbon and boron atoms (C_T = total dissolved inorganic carbon and B_T = total boron),

$$[\text{C}_T] = [\text{H}_2\text{CO}_3] + [\text{HCO}_3^-] + [\text{CO}_3^{2-}] \quad (11)$$

$$[\text{B}_T] = [\text{B}(\text{OH})_3] + [\text{B}(\text{OH})_4^-] \quad (12)$$

the 4 equations 7-10 contain 5 unknowns. The system is closed through the total alkalinity:

$$[\text{A}_T] = [\text{HCO}_3^-] + 2 \cdot [\text{CO}_3^{2-}] + [\text{B}(\text{OH})_4^-] + [\text{OH}^-] - [\text{H}^+] \quad (13)$$

Master tracers from which all reaction partners can be computed are total dissolved inorganic carbon C_T , total alkalinity A_T , and total boron B_T . C_T and A_T are advected explicitly with the velocity field. B_T is considered to be proportional to the salinity. The borate buffer accounts for about 20 % of the CO_2 buffer capacity of seawater. The phosphate and silicate buffers contributing each to about 2 % to the buffer capacity are neglected here. The concentrations of the reaction partners in (7)–(10) are coupled by the mass action law and the ionic product of water:

$$K_1 = \frac{[\text{HCO}_3^-][\text{H}^+]}{[\text{H}_2\text{CO}_3]} \quad (14)$$

$$K_2 = \frac{[\text{CO}_3^{2-}][\text{H}^+]}{[\text{HCO}_3^-]} \quad (15)$$

$$K_B = \frac{[\text{B}(\text{OH})_4^-][\text{H}^+]}{[\text{B}(\text{OH})_3]} \quad (16)$$

$$K_W = [\text{OH}^-] + [\text{H}^+] \quad (17)$$

$[H^+]$ and $[CO_3^{2-}]$ are computed from C_T and A_T using a one dimensional Newton algorithm.

2.6 GAS EXCHANGE OCEAN–ATMOSPHERE

Between the two reservoirs atmosphere and ocean surface layer CO_2 and oxygen can be exchanged. For CO_2 the following formulation is used:

$$F_{CO_2} = k_{CO_2} \cdot (pCO_{2,air} - pCO_{2,water}) \quad (18)$$

where

F_{CO_2} : carbon dioxide flux across air/sea interface

k_{CO_2} : specific gas exchange rate

For k_{CO_2} , here, a constant value of $0.063 \text{ [mol/(m}^2\cdot\text{yr}\cdot\text{ppm)]}$ is used. The CO_2 partial pressure is calculated from the free carbon dioxide concentration in seawater following Henry’s law by use of the solubility α (Weiss, 1974):

$$pCO_{2,water} = \alpha \cdot [H_2CO_3] \quad (19)$$

For oxygen, the scheme as used by Heinze et al. (1998) for CFC simulations is applied (details see description of subroutine surfch below).

3 SYSTEM DESCRIPTION

3.1 GENERAL REMARKS

The model is computed forward in time. It can either be started from initial conditions (subroutines initia, inised, bioini, and chemin) or from a previous model run making use of a restart file that contains the status of all model distributions at the end of a previous run (see statement read(83)... in the main program).

The principle flow of a model run is very simple and conventional. The program (model source code) is compiled. Several input files are read. The model is integrated. Finally output files with results are produced.

3.2 INPUT FILES

For a proper model start the following 3 files must be available in the working directory (or assigned to the respective input unit numbers as specified in the source code):

1. velocity field (file “VELOCI”)
2. grid point spacing (file “DPHILA”)
3. ocean identifiers for diagnostics (file “LANDSEACODE”)

If the model is restarted from a previous run also the corresponding restart file must be available:

restart file (file “RESTART”)

The re-start file contains the result of the preceeding model integration with all basic geochemical fields of all model reservoirs and a counter for the last year of integration. A file with exactly the same format is produced at the end of the model run (file “RESULT”, see below). If the model is run in 1-dimensional mode the formatted restart file “RESTART1D” has to be available instead of “RESTART”.

If the model results shall be compared with observations, corresponding files containing all information about observed data have to be available also. In the present version the model results can directly be compared with the GEOSECS data set (release from PACODF, Scripps Institution of Oceanography), and the CaCO_3 as well as opal sediment data sets of David Archer (<http://popeye.uchicago.edu>). The names of the observed data files are:

file name	variable
alk_geosecs_obs	alkalinity [$\mu\text{eq/kg}$]
caco3sed_obs	CaCO_3 sediment [wt.-%]
dc13_geosecs_obs	$\delta^{13}\text{C}$ of C_T [permil]
Dc14_geosecs_obs	$\Delta^{14}\text{C}$ of C_T [permil]
o2_geosecs_obs	dissolved oxygen [$\mu\text{mol/kg}$]
opalcfsed_obs	opal sediment [wt.-% on a calcite free basis]
opalsed_obs	opal sediment [wt.-% of total]
po4_geosecs_obs	phosphate [$\mu\text{mol/kg}$]
sio4_geosecs_obs	silicic acid [$\mu\text{mol/kg}$]
tco2_geosecs_obs	C_T [$\mu\text{mol/kg}$]

The velocity field file contains all information about all three velocity components, convective adjustment (convective mixing), temperature, salinity, bottom topography (land/sea-distribution, velocity points, pressure points), layer thicknesses (velocity points, pressure points) and ice cover (thickness).

In the geometry file the geographic variables for latitudinal and longitudinal size of the grid point boxes are specified. These values are not specified within the carbon cycle model to be sure of using exactly the same values as in the dynamical model.

In the input file with ocean identifiers every grid point is given a certain code that indicates which grid point lies in which ocean. The code and the corresponding ocean region are:

- 0: land
- 1: Atlantic
- 2: Pacific
- 3: Indian Ocean
- 4: North Polar Ocean

File “corrff” is read in cases that the model is newly initiated with geochemical inventories which are compatible with the GEOSECS measurements for water column tracers. Correction factors are read from this file which has the same format as file “inventories” (in fact this file has to be copied by hand on file “corrff” before new initiation with inventory adjustment).

3.3 OUTPUT FILES

Job control output (“standard output”) as produced by “print ”- and “write(,...”-statements is written to “screen”. For longer runs this file should be re-directed to a file on disc (in UNIX: `exexuctable-file > protocol-file`). The results of the model are written to a series of files. The most important is the result restart file for subsequent runs (“RESULT”, same record structure as file “RESTART”). As “RESULT” is overwritten by subsequent model runs, additionally a file “*R_run-id_timestep at end*” in the same format is written to store results of single runs. In 1-dimensional model runs the results are written sequentially as a time series from the respective grid point to file “timser1d” instead to “RESTART”.

Model results at points where observations are available (same format as observed data files such as `alk_geosecs_obs ... etc.`) are written to files:

file name	variable
<code>alk_geosecs_mod</code>	alkalinity [$\mu\text{eq/kg}$]
<code>caco3sed_mod</code>	CaCO_3 sediment [wt.-%]
<code>dc13_geosecs_mod</code>	$\delta^{13}\text{C}$ of C_T [permil]
<code>Dc14_geosecs_mod</code>	$\Delta^{14}\text{C}$ of C_T [permil]
<code>o2_geosecs_mod</code>	dissolved oxygen [$\mu\text{mol/kg}$]
<code>opalcfsed_mod</code>	opal sediment [wt.-% on a calcite free basis]
<code>opalsed_mod</code>	opal sediment [wt.-% of total]
<code>po4_geosecs_mod</code>	phosphate [$\mu\text{mol/kg}$]
<code>sio4_geosecs_mod</code>	silicic acid [$\mu\text{mol/kg}$]
<code>tco2_geosecs_mod</code>	C_T [$\mu\text{mol/kg}$]

Model results to be plotted later on in maps and cross sections are written in formatted files - for each variable one file - which can be directly used as input to the dedicated plot software. Also derived variables are written here (which do not appear in the restart file):

file name	variable
<code>alkali_plotin</code>	alkalinity, water column [$\mu\text{eq/l}$]
<code>alkas_plotin</code>	alkalinity, pore waters [$\mu\text{eq/l}$]
<code>atmos_plotin</code>	atmospheric pCO_2 [ppmv], plus $\delta^{13}\text{C}$ and $\Delta^{14}\text{C}$ [permil]
<code>bulkac_plotin</code>	bulk sediment accumulation rates [$\text{cm } (10^3 \text{ yr})^{-1}$]
<code>bulkacg_plotin</code>	bulk sediment accumulation rates [$\text{g cm}^{-2} (10^3 \text{ yr})^{-1}$]
<code>cal12sf_plotin</code>	CaCO_3 sediment [wt.-%], layerwise
<code>cal13sf_plotin</code>	$\delta^{13}\text{C}$ of CaCO_3 sediment [permil], layerwise
<code>cal14sf_plotin</code>	$\Delta^{14}\text{C}$ of CaCO_3 sediment [permil], layerwise
<code>cal12st_plotin</code>	CaCO_3 sediment [wt.-%], average over total bioturbated zone

(continued)	
file name	variable
calpoc_plotin	production rain ratio C(CaCO ₃):C(POC)
calsil_plotin	production rain ratio C(CaCO ₃):Si(opal)
claysf_plotin	inert sediment [wt.-%], layerwise
clayst_plotin	inert sediment [wt.-%], average over total bioturbated zone
co3_plotin	carbonate ion concentration, water column [$\mu\text{mol/l}$]
delco3_plotin	deviation of [CO ₃] from saturation level [$\mu\text{mol/l}$]
delta13c_plotin	$\delta^{13}\text{C}$ of C _T , water column [permil]
delta14c_plotin	$\Delta^{14}\text{C}$ of C _T , water column [permil]
oadiff_plotin	ocean-atmosphere difference in pCO ₂ [ppmv]
opacfsk_plotin	opal sediment [wt.-% on calcite free basis], layerwise
opacfst_plotin	opal sediment [wt.-% on calcite free basis], average over total bioturbated zone
opalsf_plotin	opal sediment [wt.-% of total], layerwise
opalst_plotin	opal sediment [wt.-% of total], average over total bioturbated zone
oxygen_plotin	diss. oxygen, water column [$\mu\text{mol/l}$]
oxygs_plotin	diss. oxygen, pore waters [$\mu\text{mol/l}$]
pco2surf_plotin	pCO ₂ in oceanic surface layer [ppmv]
ph_plotin	ph-value, water column
phosph_plotin	diss. phosphate, water column [$\mu\text{mol/l}$]
phosphs_plotin	diss. phosphate, pore waters [$\mu\text{mol/l}$]
poc12_plotin	suspended POC, water column [$\mu\text{mol/l}$]
poc13_plotin	$\delta^{13}\text{C}$ of suspended POC, water column [permil]
poc14_plotin	$\Delta^{14}\text{C}$ of suspended POC, water column [permil]
poc12sf_plotin	organic C sediment [wt.-%], layerwise
poc13sf_plotin	$\delta^{13}\text{C}$ of organic C sediment [permil], layerwise
poc14sf_plotin	$\Delta^{14}\text{C}$ of organic C sediment [permil], layerwise
poc12st_plotin	organic C sediment [wt.-%], average over total bioturbated zone
prcaca_plotin	CaCO ₃ export production [$\text{gC m}^{-2} \text{yr}^{-1}$]
prepho_plotin	preformed phosphate, water column [$\mu\text{mol/l}$]
prlat_plotin	growth condition parameter (POC)
prlatsi_plotin	growth condition parameter (opal)
prorca_plotin	POC export production [$\text{gC m}^{-2} \text{yr}^{-1}$]
prsili_plotin	opal export production [$\text{mol Si m}^{-2} \text{yr}^{-1}$]
sco12s_plotin	C _T , pore waters [$\mu\text{mol/l}$]
sco13s_plotin	$\delta^{13}\text{C}$ of C _T , pore waters [permil]
sco14s_plotin	$\Delta^{14}\text{C}$ of C _T , pore waters [permil]
sco212_plotin	C _T , water column [$\mu\text{mol/l}$]
seaice_plotin	sea ice thickness [m]
silcal_plotin	production rain ratio Si(opal):C(CaCO ₃)
silica_plotin	silicic acid, water column [$\mu\text{mol/l}$]
silics_plotin	silicic acid, pore waters [$\mu\text{mol/l}$]
silpoc_plotin	production rain ratio Si(opal):C(POC)
supsat_plotin	CO ₃ ²⁻ supersaturation [%]
tem_plotin	potential temperature [deg]

In the same format as the result files above, for the CaCO_3 and opal solid sediment components files are written corresponding to observations available. Only on those grid points values are defined where observations are available. A grid point is considered covered by observations if at least one measured value is within the bounds of the respective grid cell. All values are considered as vertical averages over the total local bioturbated sediment column:

file name	variable
caco3sed_pix_mod	CaCO_3 sediment [wt.-%], model result
caco3sed_pix_modobs	CaCO_3 sediment [wt.-%], model minus observation
caco3sed_pix_obs	CaCO_3 sediment [wt.-%], observation
opalcsed_pix_mod	opal sediment [wt.-% on calcite free basis], model result
opalcsed_pix_modobs	opal sediment [wt.-% on calcite free basis], model minus obs.
opalcsed_pix_obs	opal sediment [wt.-% on calcite free basis], observation
opalsed_pix_mod	opal sediment [wt.-% of total], model result
opalsed_pix_modobs	opal sediment [wt.-% of total], observation
opalsed_pix_obs	opal sediment [wt.-% of total], observation

Mean profiles of dissolved substances and their respective observed counterparts from the GEOSECS program are written to file “inventories”. This file can be used under the name “corrfl” to readjust the geochemical inventories layerwise in a subsequent run so that the model water column tracer inventories are perfectly compatible with the observed GEOSECS data at the next model run.

A number of diagnostic files are written during the model integration: “inv1_run-id.timestep at start”, “inv2_run-id.timestep at start”, and “inv3_run-id.timestep at start”, with mass conservation checks (produced by subroutine bilanz), “atpco2_run-id.timestep at start” and “runoff_run-id.timestep at start” with time series of the atmospheric pCO_2 and global sediment accumulation rates (could used also as weathering inputs in another model run), “diagno_run-id.timestep at start” with information about average tracer evolutions. Finally geometry information as needed by the plot package can be written to file “depthinfo”.

3.4 SOURCE CODE

The model source code is mainly written in FORTRAN 77. No specific vector statements are used and no external libraries are used. The code is splitted up in a suite of COMMON-Blocks, the MAIN-program, SUBROUTINES, and FUNCTIONS. The various parts of the program are listed below not in alphabetical sequence rather than in the sequence in which they are called during a model run. Important tunable parameters were extracted from the source code into a NAMELIST so that they can be changed without recompilation of the source code. The source code is written under the assumption that it is used with the make utility and corresponding preprocessing (see chapter on SOURCE CODE ADMINISTRATION below). Different model configurations are specified through compiler options. A 1-dimensional model torso with prognostic sediment part only can

be activated by choosing compiler option “resta1d” (see below in section HOW TO RUN THE MODEL within chapter USER’S GUIDE). The various model parts are described in more detail in the following paragraphs.

3.4.1 COMMON-Blocks

Three sets of COMMON-blocks are specified and summarized in the three files “com_block.h”, “com_v12mnmt.h”, and “com_sed.h”. File “com_block.h” contains all parameters and variables for the water column part of the model. Also “com_v12mnmt.h” belongs to the water column part. Mnemotechnically easier variable names are specified here for the water column tracer concentration arrays. All parameters and arrays which are used in the sediment model routines are summarised in file “com_sed.h”.

For indices of the 2-, 3-, and 4-dimensional arrays the following notation is used throughout the model:

- i: zonal direction, water column and sediment
- j: meridional direction, water column and sediment
- k: vertical direction, water column
- ks: vertical direction, sediment
- iv: tracer species, water column
- iva: tracer species, atmosphere
- ivs: tracer species, sediment

The array boundaries corresponding to these indices are specified in parameter statements:

- ie: zonal direction, water column and sediment
- je: meridional direction, water column and sediment
- ke: vertical direction, water column
- kse: vertical direction, sediment
- nv: tracer species, water column
- nva: tracer species, atmosphere
- nvsol, nvwat: tracer species, sediment (solid components, pore waters)

The advection algorithm needs four latitude bands more (two at the northern and two at the southern fringe) than are actually valid for the model region. The first (beginning from north to south) and last latitude bands that are valid for the model domain and the geochemical variables (without dummies) are specified by:

- jl1: first latitude band index (northern fringe of model domain) that contains valid information for the chemical variables
- jle: last latitude band index (southern fringe of model domain) that contains valid information for the chemical variables

An overview on the most important predictive variables is given in the tables following below.

Atmosphere (“com_block.h”, “com_v12mnmt.h”)

quantity	variable	do loop variable (equivalenced)
$^{12}\text{CO}_2$	atc12(i,j)	atc(i,j,1)
$^{13}\text{CO}_2$	atc13(i,j)	atc(i,j,2)
$^{14}\text{CO}_2$	atc14(i,j)	atc(i,j,3)
oxygen	o2at(i,j)	atc(i,j,4)

Ocean water column (“com_block.h”, “com_v12mnmt.h”)

quantity	variable	do loop variable (equivalenced)
C_T	sco212(i,j,k)	ca(i,j,k,1)
alkalinity	alkali(i,j,k)	ca(i,j,k,2)
phosphate	phosph(i,j,k)	ca(i,j,k,3)
oxygen	oxygen(i,j,k)	ca(i,j,k,4)
suspended POC	poc12(i,j,k)	ca(i,j,k,5)
silicic acid	silica(i,j,k)	ca(i,j,k,6)
DI^{13}C	sco213(i,j,k)	ca(i,j,k,7)
DI^{14}C	sco214(i,j,k)	ca(i,j,k,8)
PO^{13}C	poc13(i,j,k)	ca(i,j,k,9)
PO^{14}C	poc14(i,j,k)	ca(i,j,k,10)

Bioturbated sediment, pore water components (“com_sed.h”)

quantity	variable	do loop variable (equivalenced)
C_T	sco12s(i,j,ks)	wca(i,j,ks,1)
oxygen	oxygs(i,j,ks)	wca(i,j,ks,2)
silicic acid	silics(i,j,ks)	wca(i,j,ks,3)
alkalinity	alkas(i,j,ks)	wca(i,j,ks,4)
phosphate	phosphs(i,j,ks)	wca(i,j,ks,5)
DI^{13}C	sco13s(i,j,ks)	wca(i,j,ks,6)
DI^{14}C	sco14s(i,j,ks)	wca(i,j,ks,7)

Bioturbated sediment, solid sediment components (“com_sed.h”)

quantity	variable	do loop variable (equivalenced)
CaCO_3	cal12sf(i,j,ks)	casf(i,j,ks,1)
organic C	poc12sf(i,j,ks)	casf(i,j,ks,2)
opal	opalsf(i,j,ks)	casf(i,j,ks,3)
inert material	claysf(i,j,ks)	casf(i,j,ks,4)
$\text{Ca}^{13}\text{CO}_3$	cal13sf(i,j,ks)	casf(i,j,ks,5)
PO^{13}C	poc13sf(i,j,ks)	casf(i,j,ks,6)
$\text{Ca}^{14}\text{CO}_3$	cal14sf(i,j,ks)	casf(i,j,ks,7)
PO^{14}C	poc14sf(i,j,ks)	casf(i,j,ks,8)

Also for some other quantities equivalenced mnemotechnical variable names and corresponding do loop variables are used. Throughout the source code the implicit type

convention is used with variables beginning with a-h, o-z being of type REAL, and variables beginning with i-n being of type INTEGER. Variables of type CHARACTER and LOGICAL are defined explicitly if necessary.

3.4.2 MAIN Program

The main program ‘hamocc2s’ (“main.F”) is divided into three parts:

- initiation and input
- time stepping loop
- output

Most of the computing time is used within the time stepping loop. The different biogeochemical and physical processes are simulated subsequently in separate routines (“time splitting method”) that are all part of the time loop. Only the advection algorithm (transport of substances with the ocean velocity field) and the extraction of biolimiting nutrient from the surface layer are carried out parallel in one subroutine.

The following files are opened for input and output:

unit No.	file name	input or output
11	<i>inv1_run-id_timestep at start</i>	output
12	<i>inv2_run-id_timestep at start</i>	output
13	<i>inv3_run-id_timestep at start</i>	output
15	RESTART1D	input/output depending on compiler option
17	LANDSEACODE	input
38	VELOCI	input
38	VELOCI_neu	input (used additionally for ke=22)
42	<i>atpco2_run-id_timestep at start</i>	output
44	<i>runoff_run-id_timestep at start</i>	output
61	*_geosecs_obs	input
62	*_geosecs_mod	output
63	*_pix_obs	output
64	*_pix_mod	output
65	*_pix_modobs	output
78	timser1d	output
70	*_plotin	output
79	corrf	input
82	<i>diagno_run-id_timestep at start</i>	output
83	RESTART	input
86	inventories	output
85	<i>R_run-id_timestep at start</i>	output
87	RESULT	output
97	depthinfo	output

3.4.3 SUBROUTINE resta1d

This subroutine is called only for the 1-dimensional case. All variables, which are necessary for a restart of the model are read from a formatted restart file “RESTART1D” (unit=15). Only information for one single profile is extracted from the 2- and 3-dimensional arrays stored in RESTART1D. The zonal and meridional indices for the respective grid point are set in the namelist (variables id1 and jd1).

3.4.4 SUBROUTINE initia

In initia all variables are initiated except those for the sediment part of the model. If the model is not started from a restart run, but rather from basic initial conditions, these are set here for the water column and the atmosphere. The velocity and thermohaline fields are read through subroutine reacir, while the biological and chemical variables and constants are set by subroutines bioini and chemin. Further all geometric variables (topography, layer thicknesses) and the meridional diffusive atmospheric tracer transport are initiated here.

If the model is integrated for the 22 layer case, also the explicit vertical diffusion algorithm for the water column is prepared. Coefficients for vertical diffusion are computed in proportion to the local vertical density gradient. In order to determine the in situ density the potential temperature values as given by the LSG-OGCM are converted to in situ temperatures in function tinsit.

3.4.5 SUBROUTINE reacir

The annual mean values of the 3-dimensional velocity field, potential temperature, salinity, water depth as well as layer thicknesses at u- and p-points, sea ice thickness, and convective adjustment, all as provided by a previous run with the dynamical LSG-OGCM are read. All variables containing length values are converted from m to cm. A check for completeness of the data read is carried out. This subroutine should not be touched by the user.

3.4.6 FUNCTION tinsit

Tinsit computes the in situ temperature $T(p)$ from the potential temperature Θ through inversion of the formula for computation of Θ from $T(p)$ after Bryden (1973). The inversion calculation is carried out through a Newton iteration. The original version of this subroutine was provided for the HOPE ocean model and transferred to the geochemical model later on.

3.4.7 SUBROUTINE bioini

Here the initiation of all biological and biogeochemical variables for the water column part of the model is carried out. In particular the parametrisation for the particle flux through the water column and the growth conditions for plankton are specified.

3.4.8 SUBROUTINE chemin

All constants and variables concerning inorganic chemical reactions are set here such as the dissociation constants for carbonic and boric acid as well as the solubilities of oxygen and CaCO_3 in sea water. Pressure correction is computed for chemical equilibrium constants if necessary.

3.4.9 FUNCTION rho

The equation of state for sea water is solved for density as a function of salinity, temperature and pressure by applying the method as described in UNESCO (1983).

3.4.10 SUBROUTINE inised

All geochemical constants and variables for the sediment part are specified here. Also the geometry of the sediment is defined here (layer thicknesses, porosities). In case of a fundamental new start of the model (no restart from a previous run) the model starts with a homogeneous layer of clay material and no biogenic sediment components at all.

3.4.11 SUBROUTINE bilanz

This is a diagnostic subroutine. It can be called at almost every position within the model code (between the treatment of different processes and outside do loops, of course,) in order to integrate all tracer inventories over all model reservoirs for a check of mass conservation within the entire model system.

3.4.12 SUBROUTINE positio

Positio provides geographical longitude and latitude values in degrees for every grid point of the model. The position specification is identical to that as given for the LSG-OGCM in Maier-Reimer et al. (1993). The northernmost latitude value is at $+88.75^\circ$ (88.75°N , $j=3$), the southernmost at -88.75° (88.75°S , $j=74$). The longitude for index $i=1$ is -1.25° (1.25°W) for $j=3$, shifting 2.5 degrees westward per index j going southward with an increment of 2.5° (i.e. point $i=1$, $j=4$ is at -3.75°W , 86.25°N , etc...). In each zonal band the increment for longitudes is 5° . Eastern longitudes and northern latitudes are positive.

3.4.13 SUBROUTINE co3waco

Here the carbonate ion and proton concentrations (convertable to pH-value) are computed. Both variables are derived from C_T and A_T . With the help of the mass action laws for the dissociation of carbonic and boric acid C_T and A_T can be written as expressions of the only chemical variables $h = [H^+]$ and $s = [CO_2]$ (Maier-Reimer and Hasselmann,

$$C_T = s \left(1 + \frac{K_1}{h} + \frac{K_1 K_2}{h^2} \right) \quad (20)$$

$$A_T = s \left(\frac{K_1}{h} + 2 \frac{K_1 K_2}{h^2} \right) + \frac{K_w}{h} + \frac{B_T}{(1 + h/K_b)} - h \quad (21)$$

Substituting s in (21) with (20) yields a nonlinear equation which depends on h only.

$$A_T = \frac{C_T}{(1 + K_1/h + K_1 K_2/h^2)} \cdot \left(\frac{K_1}{h} + 2 \frac{K_1 K_2}{h^2} \right) + \frac{K_w}{h} + \frac{B_T}{(1 + h/K_b)} - h \quad (22)$$

For the correct h the following function of h has to be zero:

$$f(h) = A_T - \frac{C_T}{(1 + K_1/h + K_1 K_2/h^2)} \cdot \left(\frac{K_1}{h} + 2 \frac{K_1 K_2}{h^2} \right) + \frac{K_w}{h} + \frac{B_T}{(1 + h/K_b)} - h \quad (23)$$

The appropriate h is determined from setting (23) to zero and solved numerically for h through a 1-dimensional Newton algorithm. The carbonate ion concentration finally is determined from inserting the value for s (found by substituting the solution for h from (23) in (20) in the mass action law for the second dissociation step of carbonic acid (15).

3.4.14 SUBROUTINE biopro

The export production rates of POC and opal are computed within the advection algorithm (subroutine advect) (see eqs. 44 and 2 in the chapters TRANSPORT OF TRACERS WITH OCEAN VELOCITY FIELD and BIOLOGICAL PRODUCTION OF PARTICULATE MATTER above). In subroutine biopro the CaCO_3 export production is determined according to (3) and (4) and the vertical redistribution of biogenic particulate matter through a parameterisation of the vertical particle flux is performed. Corresponding flux profiles are initiated in subroutine biopro while the e-folding depths (depth levels where particle flux through the water column is reduced to $1/e$ of the export production) are specified externally in a namelist.

3.4.15 SUBROUTINE updrai

In updrai the particle rain arrays to the ocean floor are updated, i.e. the sediment deposition is computed. Here also the dissolved tracer concentrations in the uppermost compartment (the lowermost wet water column box) for the vertical pore water diffusion are set to the actual bottom water values.

3.4.16 SUBROUTINE dissol3

Here the porewater diffusion of dissolved tracers within the sediment column and the pore water chemistry (dissolution of opal and CaCO_3 , remineralisation of POC) are computed

simultaneously. The solid components S and dissolved components P are coupled with each other by the reaction rate. Rather than computing directly the diffusion of the dissolved substance, here, the diffusive transport of the respective undersaturations (or deviations from saturation concentration) simultaneously with the reduction of undersaturation due to chemical pore water reactions are determined with an implicit numerical method:

$$\frac{dU}{dt} = \frac{\partial}{\partial z} \left(D_W \frac{\partial U}{\partial z} \right) - G \quad (24)$$

where

U : undersaturation (deviation from saturation concentration)

G : reaction rate (sink of undersaturation from dissolution of solid material)

D_W : diffusion coefficient for pore water diffusion.

Since the undersaturations are positively definite no negative concentrations for the solid components can result regardless of time step and reaction kinetics. The change of a solid sediment component due to pore water reactions and particle deposition is corresponding to (24):

$$\frac{dS_*}{dt} = -G + Q \quad (25)$$

where

S_* : solid sediment component expressed in the same units as U

G : reaction rate (sink due to dissolution)

Q : gain from particle rain.

The amount of matter subject to dissolution G per unit time depends on the reactivity r_c^* , the undersaturation U , and the amount of solid material available S_* :

$$G = r_c^* \cdot U \cdot S_* \quad (26)$$

where the reactivity r_c^* is:

$$r_c^* = \frac{r_c}{P_{sat}} \quad (27)$$

with

r_c : reaction rate [1/unit time]

P_{sat} : saturation concentration in solution

In discretised form (25) becomes:

$$\frac{S_*^{t+\Delta t} - S_*^t}{\Delta t} = -r_c^* \cdot U^{t+\Delta t} \cdot S_*^{t+\Delta t} + Q \quad (28)$$

With the approximation:

$$r_c^* \cdot U^{t+\Delta t} \approx r_c^* \cdot U^t \quad (29)$$

the solid concentration $S_*^{t+\Delta t}$ can be substituted in the G -term of (24) as a first guess (the approximation introduces formally a deviation from the reaction rate which has been chosen, if the system is far away from equilibrium; this is not considered as critical):

$$S_*^{t+\Delta t}_{first\ guess} = \frac{S_*^t + Q \cdot \Delta t}{1 + \Delta t \cdot r_c^* \cdot U^t} \quad (30)$$

Schematically written, (24) is then solved numerically from:

$$\begin{aligned} \frac{U^{t+\Delta t} - U^t}{\Delta t} = & \frac{D_w^{upper}(U_{upper}^{t+\Delta t} - U^{t+\Delta t}) - D_w^{lower}(U^{t+\Delta t} - U_{lower}^{t+\Delta t})}{2\Delta x^2} \\ & - \frac{r_c^* \cdot U^{t+\Delta t} \cdot (S_*^t + Q \cdot \Delta t)}{1 + \Delta t \cdot r_c^* \cdot U^t} \end{aligned} \quad (31)$$

Scheme (31) leads to a tridiagonal system of equations which can be readily solved by standard procedures. The porewater concentrations and solid sediment concentrations after the diffusion-reaction step then become:

$$P^{t+\Delta t} = P_{sat} - U^{t+\Delta t} \quad (32)$$

$$S_*^{t+\Delta t} = S_*^t - \Delta t \cdot r_c^* \cdot U^{t+\Delta t} \cdot \frac{S_*^t + Q \cdot \Delta t}{1 + \Delta t \cdot r_c^* \cdot U^{t+\Delta t}} + \Delta t \cdot Q \quad (33)$$

The different chemical species are treated in the following sequence:

1. The clay fraction is added from particle rain (no reaction implemented so far).
2. Opal rain and redissolution plus silicic acid pore water diffusion are performed.
3. POC rain, remineralisation, and pore water diffusion of oxygen and phosphate are carried out. The corresponding changes in C_T and A_T are stored. The change in porewater CO_3^{2-} due to POC decay is computed.
4. CaCO_3 particle deposition and dissolution are computed where the degree of pore-water saturation is approximated from the pore water values of A_T and C_T at the old time levels plus the CO_3 reduction from POC remineralisation.
5. Finally pore water diffusion of C_T and A_T is carried out (assuming constant pore water diffusion coefficients for all carbon species).

The vertical advection of sediment material and bioturbation are computed in separate subroutines (solid2 and biotur).

3.4.17 SUBROUTINE co3powa

This routine updates the pore water values of H^+ (pH-value) and CO_3^{2-} with the same method as used for the open water column (see description of subroutine co3waco above).

3.4.18 SUBROUTINE lefttha

Computes the left hand side of the tridiagonal system of linear equations for the computation of the new undersaturations in the pore waters according to (31). In contrast to the simplified scheme in (31) also variable grid point spacings and porosities are accounted for.

3.4.19 SUBROUTINE tridvec

This routine solves scheme (31) for the pore water undersaturations after diffusion and recations using 2-dimensional arrays (running along the zonal bands in the innermost loop for effective vectorisation).

3.4.20 SUBROUTINE solid2

Here, the vertical advection of solid sediment components is carried out and sediment accumulation rates are determined. The entire bioturbated sediment mixed layer and all layers are assumed to have constant geometry, i.e., do not change their thickness. Therefore the sediment column has to be shifted vertically due to gain of material from particle deposition out of the water column and loss from redissolution of solid material within the sediment layer (“gaps” in the sediment which are produced due to chemical erosion). Three different cases are considered:

1. The deposition onto the uppermost sediment layer exceeds redissolution and remineralisation within the entire sediment column at one grid point. In this case solid material is accumulated and vanishes from the system down below the lowermost sediment layer into “diagenetically consolidated” material of the lithosphere.
2. No particle deposition occurs (e.g., due to a change in the velocity field and an associated shift of the sea ice cover) but chemical erosion of previously deposited material continues. No sediment accumulation occurs and the gaps within the sediment are filled with material from below. Material brought up into the lowermost sediment layer is considered inert as an approximation (i.e. only clay is advected upward from the “lithosphere” into the mixed layer).
3. Particle deposition exceeds re-dissolution of the uppermost sediment layer, but is smaller than the decay of material in the entire local sediment column. Then sediment advection changes its sign somewhere within the bioturbated zone. No solid material is accumulated.

After subroutine “solid2” the sediment mixed layer is again completely filled with solid material except for the pore water volumes as specified in subroutine inised. The resulting accumulation rates can be used in globally integrated form for comparison with the global terrestrial input rates as specified in the namelist in order to estimate how far away from equilibrium the model is.

3.4.21 SUBROUTINE weath

Input from terrestrial sources is added homogeneously to the ocean surface layer in dissolved form in order to balance the loss of matter from the system due to accumulation of solid sediment (loss to the “lithosphere”).

3.4.22 SUBROUTINE bioturs

Bioturbation is modelled as diffusion of the solid sediment components using the same numerical method as used for the pore water diffusion. The only difference is that the sediment column is considered closed at its base for bioturbation while for pore water diffusion a zero gradient across the sediment/“solid lithosphere”-boundary is assumed.

3.4.23 SUBROUTINE tridia

Solves the system of linear equations for the determination of the solid sediment components after bioturbation.

3.4.24 SUBROUTINE oxycon

POC is remineralised with a given rate constant (variable remira) as long as sufficient oxygen (variable oxymin) is available. This routine applies for the water column only (organic carbon degradation within the bioturbated sediment is treated in subroutine dissol3).

3.4.25 SUBROUTINE surfch

This subroutine computes the gas exchange between ocean and atmosphere. In this version of the model a constant gas transfer velocity is used. The oceanic surface H_2CO_3 values are computed from C_T and A_T by a two dimensional Newton algorithm. Because the timescale for the equilibration of the surface layer and tropospheric air with respect to CO_2 is shorter than the time step of one year, an explicit numerical scheme here would lead to artificially high gas transfer rates. Therefore, the gas transfer rates are computed with an implicit method. In general the CO_2 flux F across the air sea interface into the atmosphere is:

$$F = \gamma(P_o - P_a) \quad (34)$$

where

- F : upward flux, e.g. in $[\text{mol m}^{-2} \text{ yr}^{-1}]$
- γ : specific gas transfer rate, e.g. in $[\text{mol m}^{-2} \text{ yr}^{-1} \text{ ppm}^{-1}]$
- P_a : pCO_2 in the atmosphere [ppm]
- P_o : pCO_2 in the ocean surface layer [ppm]

In discretised form the change in atmospheric pCO₂ per time step (1 year) is approximated through a flux resulting from a mean pCO₂ gradient averaged from the gradients at the old and new time levels:

$$P_a^{t+\Delta t} - P_a^t = V^{-1} \cdot 0.5 \cdot (F^{t+\Delta t} + F^t) \quad (35)$$

$$\Leftrightarrow P_a^{t+\Delta t} - P_a^t = \frac{\gamma}{V \cdot 2} (P_o^{t+\Delta t} + P_o^t - P_a^{t+\Delta t} - P_a^t) \quad (36)$$

$$\Leftrightarrow P_a^{t+\Delta t} = \frac{P_a^t [1 - \gamma/(2 \cdot V)] + [\gamma/(2 \cdot V \cdot \alpha)] (S^{t+\Delta t} + S^t)}{[1 + \gamma/(2 \cdot V)]} \quad (37)$$

$$(38)$$

where

V : conversion factor for moles/l in ocean to ppmv in atmosphere

α : solubility of CO₂ in seawater

$S^{t+\Delta t}, S^t$: ocean surface [H₂CO₃] at new and old time levels

$S^{t+\Delta t}$ (as well as the proton concentration $h^{t+\Delta t}$ at the new time step) is computed through a two-dimensional Newton algorithm (confer also eqs. 20-23 for an equivalent procedure) from:

$$\begin{aligned} C_T^t + V P_a^t &= C_T^{t+\Delta t} + V P_a^{t+\Delta t} \\ \Leftrightarrow C_T^t + V P_a^t &= S^{t+\Delta t} \left(1 + \frac{K_1}{h^{t+\Delta t}} + \frac{K_1 K_2}{(h^{t+\Delta t})^2} \right) \\ &\quad + V \cdot \frac{P_a^t [1 - \gamma/(2 \cdot V)] + [\gamma/(2 \cdot V \cdot \alpha)] (S^{t+\Delta t} + S^t)}{[1 + \gamma/(2 \cdot V)]} \end{aligned} \quad (39)$$

Finally, in an explicit step using the intermediate CO₂ flux rates between the old and new time level, the actual atmospheric pCO₂ and ocean C_T levels after gas exchange are computed:

$$\begin{aligned} F_{up} &= \gamma \frac{S^{t+\Delta t} + S^t}{2 \cdot \alpha} \\ F_{down} &= \gamma \frac{P_a^{t+\Delta t} + P_a^t}{2} \\ P_a^{t+\Delta t} &= P_a^t + F_{up} - F_{down} \end{aligned} \quad (40)$$

$$C_T^{t+\Delta t} = C_T^t - V(F_{up} - F_{down}) \quad (41)$$

Gas exchange for oxygen is performed separately with special treatment at points where deep vertical convection occurs. In general we have for the change of oxygen concentration in water due to gas exchange:

$$\frac{dC}{dt} = F_{O_2}/\Delta z, \quad (42)$$

where

C : concentration of dissolved oxygen in water
 F_{O_2} : flux of oxygen across the air/sea interface
 into a layer of thickness Δz

The numerical scheme for the oceanic oxygen concentration at the new time level is then (according to the analytical solution of (42)):

$$C^{t+\Delta t} = C_{equilibrium} + (C^t - C_{equilibrium}) \cdot e^{(-k_{av}/\Delta z) \cdot \Delta t} \quad (43)$$

with

$C^{t+\Delta t}$: oceanic O_2 concentration at new time level
 C^t : oceanic O_2 concentration at old time level
 $C_{equilibrium}$: oceanic O_2 concentration for solubility equilibrium
 k_{av} : gas transfer velocity
 Δz : thickness of surface layer,
 which takes directly part in gas exchange
 Δt : time step

In cases of hydrostatic stability, Δz is the standard layer thickness of the uppermost model layer, while at grid points with convective overturning, Δz is extended to the entire depth interval of the unstable part in the water column.

3.4.26 SUBROUTINE advect

The tracer equation (1) is formulated with an upstream scheme:

$$\frac{c^{t+\Delta t} - c^t}{\Delta t} = - \sum_i v_i \cdot \frac{c_i^{t+\Delta t} - c^{t+\Delta t}}{\Delta x_i} + A_{conv.adj.} \cdot (c^{t+\Delta t} - c_{lower\ layer}^{t+\Delta t}) - aI \frac{V_{max}(c^{t+\Delta t})^2}{K_s + c^{t+\Delta t}} \quad (44)$$

where

c : tracer concentration
 t : previous time level
 $t + \Delta t$: new time level
 v_i : velocity component (zonal, meridional, vertical)
 $A_{conv.adj.}$: convective adjustment (not zero in case of hydrostatic instability)
 a : 1 if c is dissolved phosphate or silicic acid, 0 else
 I : parameter describing growth conditions for phytoplankton
 V_{max} : maximum velocity of nutrient uptake
 K_s : half saturation constant (nutrient concentration where $dc/dt = V_{max}/2$)

The advection equation is solved iteratively using a single-level scheme. An exactly mass conserving method is used which is described in a highly simplified manner below. Let us consider a central grid box with concentrations c^t and $c^{t+\Delta t}$ at the old and new time levels respectively. Two neighboring boxes on the left and right side of the central box have the concentrations $c_l^{t+\Delta t}$ and $c_r^{t+\Delta t}$ at the new time level. Per time step the left and right boxes exchange A_l and A_r parts of their box volume (which is constant for all boxes in this example). The concentration in the central box at the new time level can then be computed from

$$c^{t+\Delta t} - c^t = A_l(c_l^{t+\Delta t} - c^{t+\Delta t}) + A_r(c_r^{t+\Delta t} - c^{t+\Delta t}) \quad (45)$$

At first, however, the approximate solution for $c^{t+\Delta t}$ is determined through iteration of:

$$c^{t+\Delta t}(1 + A_l + A_r) = c^t + A_l c_l^{t+\Delta t} + A_r c_r^{t+\Delta t} \quad (46)$$

This approximate solution of (46) is then introduced into the righthand side of (45). Therefore, all fluxes of the approximate solution balance each other globally and locally exactly for the final result $c^{t+\Delta t}$.

3.4.27 SUBROUTINE atmdif

Meridional diffusive transport of atmospheric gases (CO₂, oxygen) is carried out after computation of zonal average concentrations. This procedure is based on the short hemispheric mixing times of few weeks for tropospheric air and the long time step of the model.

3.4.28 SUBROUTINE raddec

The sink of ¹⁴C due to radioactive decay is performed here for all radiocarbon containing substances in all model reservoirs. A corresponding source of ¹⁴C is added homogeneously to the atmosphere.

3.4.29 SUBROUTINE pools

This is a diagnostic subroutine which provides global bulk figures of interest such as the global export production rates of biogenic matter.

3.4.30 SUBROUTINE calib

This routine converts the notation of the computed ¹³C and ¹⁴C so that the model output can directly be compared with $\delta^{13}\text{C}$ and $\Delta^{14}\text{C}$ data. (For all carbon interactions, always total carbon is considered neglecting the effect of radioactive decay of the small ¹⁴C fraction. The model inventories of ¹³C and ¹⁴C are thus also fixed by the calibration at the end of the model run. For a subsequent model restart all ¹³C and ¹⁴C are written in uncalibrated form onto the respective restart file.)

3.4.31 SUBROUTINE modobs

All subroutine calls for a comparison of model results with observations for different tracers and different reservoirs are carried out from this subroutine.

3.4.32 SUBROUTINE mowaco

This routine compares model results for water column tracers with observed values. All model values are interpolated onto the position and depth level of the observation. Integral

values of observations and model results are computed for the different model layers for those points at which observations are available (these mean profiles can be used for a quick look comparison of modelled and observed global mean tracer profiles).

3.4.33 SUBROUTINE mowaff

This routine compares model results for particle fluxes through the water column with observed values from sediment trap values. All model values are interpolated onto the position and depth level of the observation. Observed data have to be provided by the respective user. In the present model version this routine is not called but may be activated on request.

3.4.34 SUBROUTINE mosoli

This routine compares model results for solid sediment components. All model values are interpolated onto the position of the observation. In general only averages of the entire bioturbated sediment column are compared here.

3.4.35 SUBROUTINE sedint

Layerwise model results for solid sediment component are integrated over the entire thickness of the bioturbated sediment mixed layer of the model. Opal is given in two different units: as weight percentage of total sediment and as weight percentage of sediment on a calcite free basis.

3.4.36 SUBROUTINE outwri

Formatted output files are generated which serve as input to the post processing software. Derived variables are also computed for diagnostic purposes. In all formatted output files undefined variables (such as ocean variables at land points) are set to $-.1111\text{E}+11$, a number which probably never occurs in oceanography.

3.5 SOURCE CODE ADMINISTRATION

All program parts are combined and compiled using the “make” command including code preprocessing where the parameter statements and common blocks are glued into the respective program parts through a “#include” command. Therefore, parameter statements and common blocks have to be held only once which facilitates an update of the source code significantly. Different model configurations (such as different numbers of tracers) are provided by compiler options (“#ifdef”s within the source code).

3.6 NAMELIST PARAMETERS

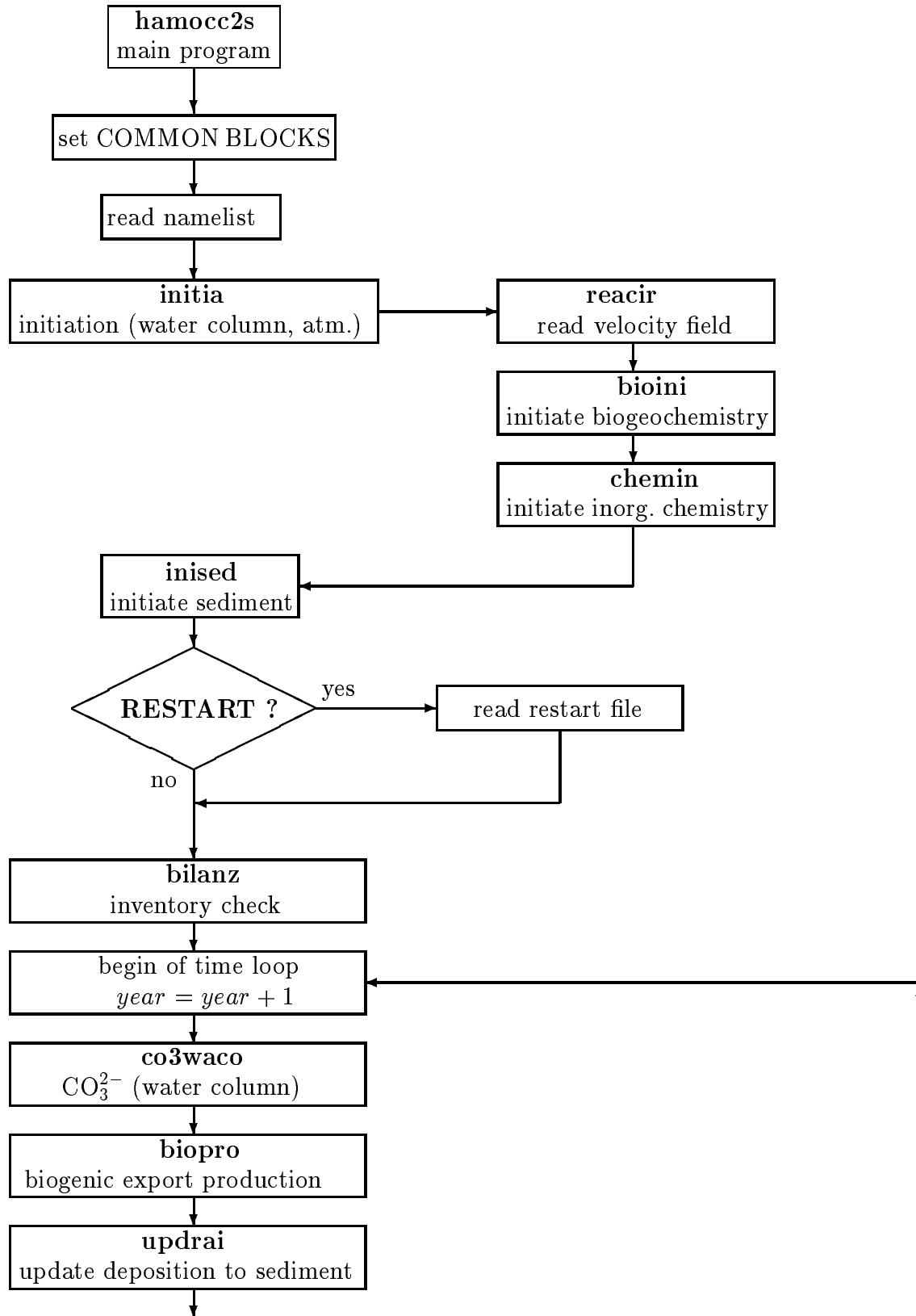
Tunable constants of the model and parameters for carrying out a model integration are set in a namelist externally from the source code. Thus, the model can be run for a considerable number of experiments without touching or recompiling the program text. The namelist, however, belongs directly to the source code. With a change in the namlist values compared to the one associated with this documented version, different and unwanted results may occur.

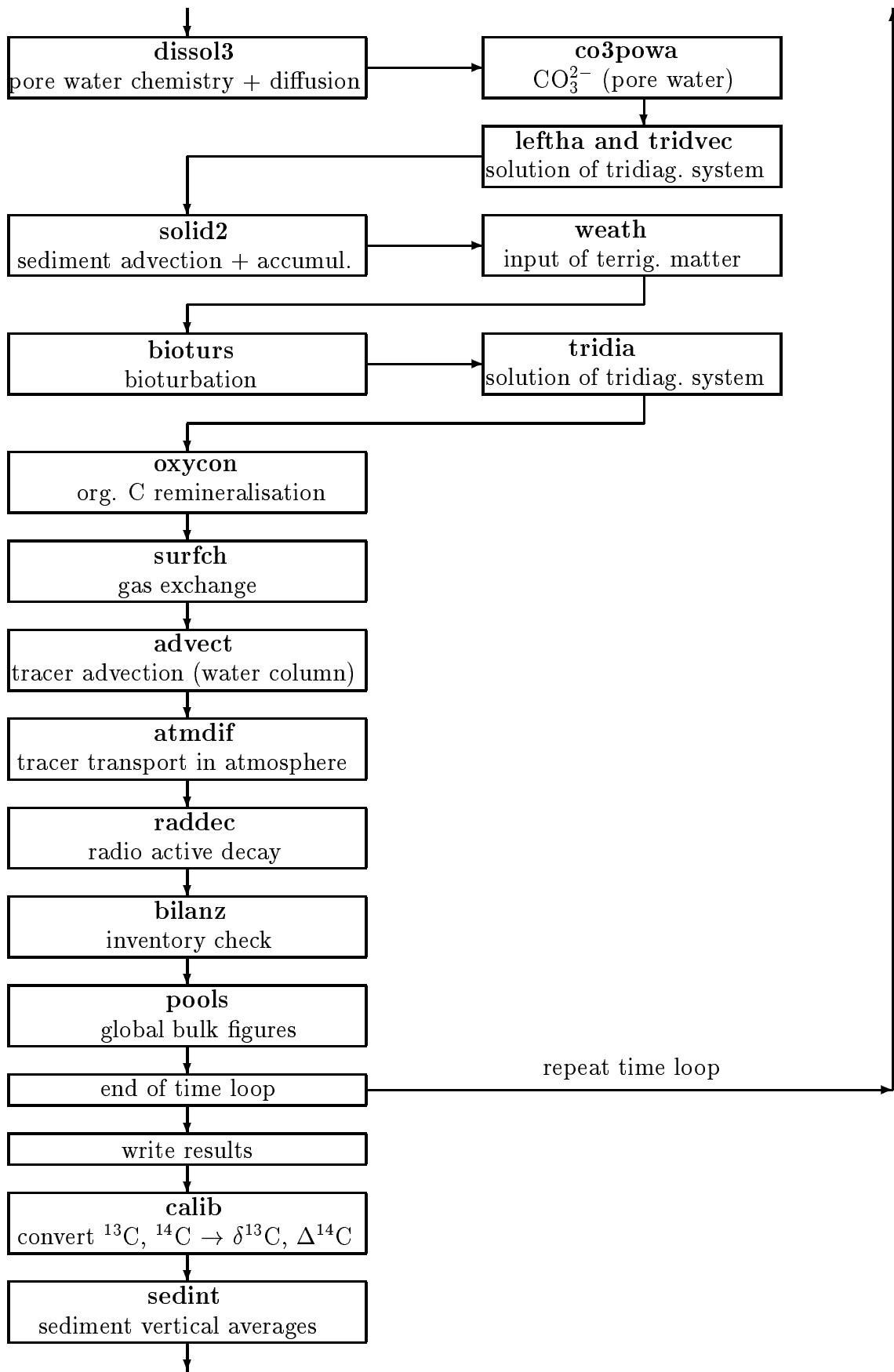
The following constants are set in the namelist:

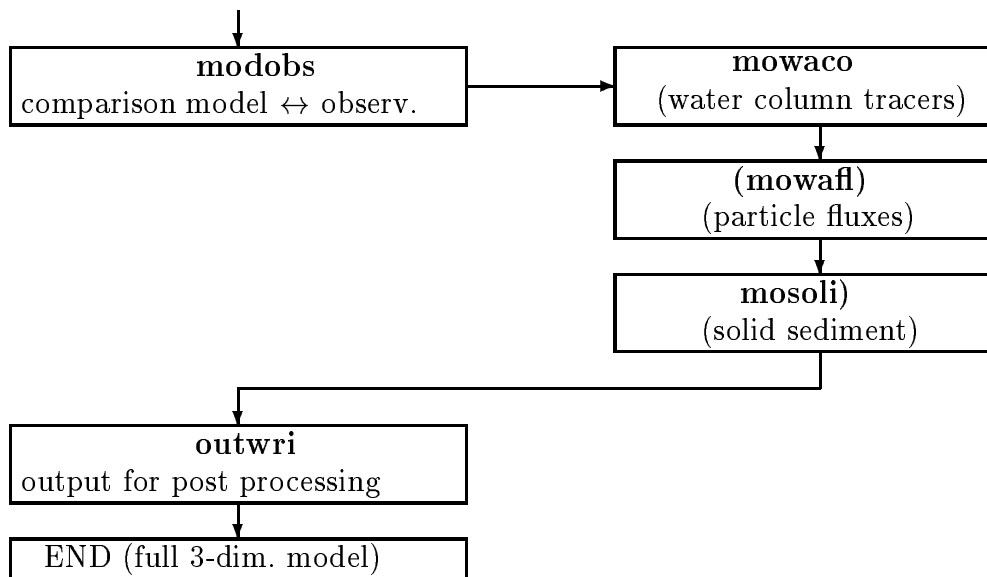
name of constant	declared type	description
intstp	INTEGER	number of timesteps to be integrated
timax	REAL	threshold for CPU time to be used up per run
runid	CHARACTER	name of run
ifulbi	INTEGER	1 → mass balance check after each subr.
iyear0	INTEGER	1 → start year is set to nyear0
nyear0	INTEGER	integer number of year if iyear.eq.1
irstart	INTEGER	1 → run continued on basis of re-start file
iinvad	INTEGER	inventories are adjusted accord. to observations
isedini	INTEGER	1 → sediment is set to 100 % clay at each start
conc0	REAL	half saturation constant for PO_4^{3-} uptake
cosi0	REAL	half saturation constant for of $\text{Si}(\text{OH})_4$ uptake
pendeo	REAL	penetration depth for POC
pendec	REAL	penetration depth for CaCO_3
pendes	REAL	penetration depth for opal
caco3r	REAL	maximum of local rain ratio $\text{C}(\text{POC}):\text{C}(\text{CaCO}_3)$
calthre	REAL	opal-production/POC-production threshold value for CaCO_3 -production
dustflu	REAL	aeolian dustflux to ocean in $\text{g}/(\text{m}^2)$
sisat	REAL	pore water $\text{Si}(\text{OH})_4$ sat. value for opal in mole/l
rcorg	REAL	pore water rate constant for POC remineralisation
rccal	REAL	pore water rate constant for CaCO_3 redissolution
rcopal	REAL	pore water rate constant for opal redissolution
sublth	REAL	sublayer thickness above sediment water interface
biotdb	REAL	bioturbation coefficient $\text{cm}^2/1000\text{yr}$
id1	INTEGER	zonal index of grid point for 1-dim. version
jd1	INTEGER	meridional index of grid point for 1-dim. version
slc12p	REAL	weathering flux of C_T [10^{12} moles C/year]
slc13p	REAL	weathering flux of ^{13}C [10^{12} moles C/year]
slc14p	REAL	weathering flux of ^{14}C [10^{12} moles C/year]
slalkp	REAL	weathering flux of A_T [10^{12} equivalents/year]
slpo4	REAL	weathering flux of PO_4^{3-} [10^{12} C:P moles P /year] corresp. to POC influx in [10^{12} moles C /year]
slopalp	REAL	weathering flux of $\text{Si}(\text{OH})_4$ [10^{12} moles Si/year]

3.7 FLOW CHARTS

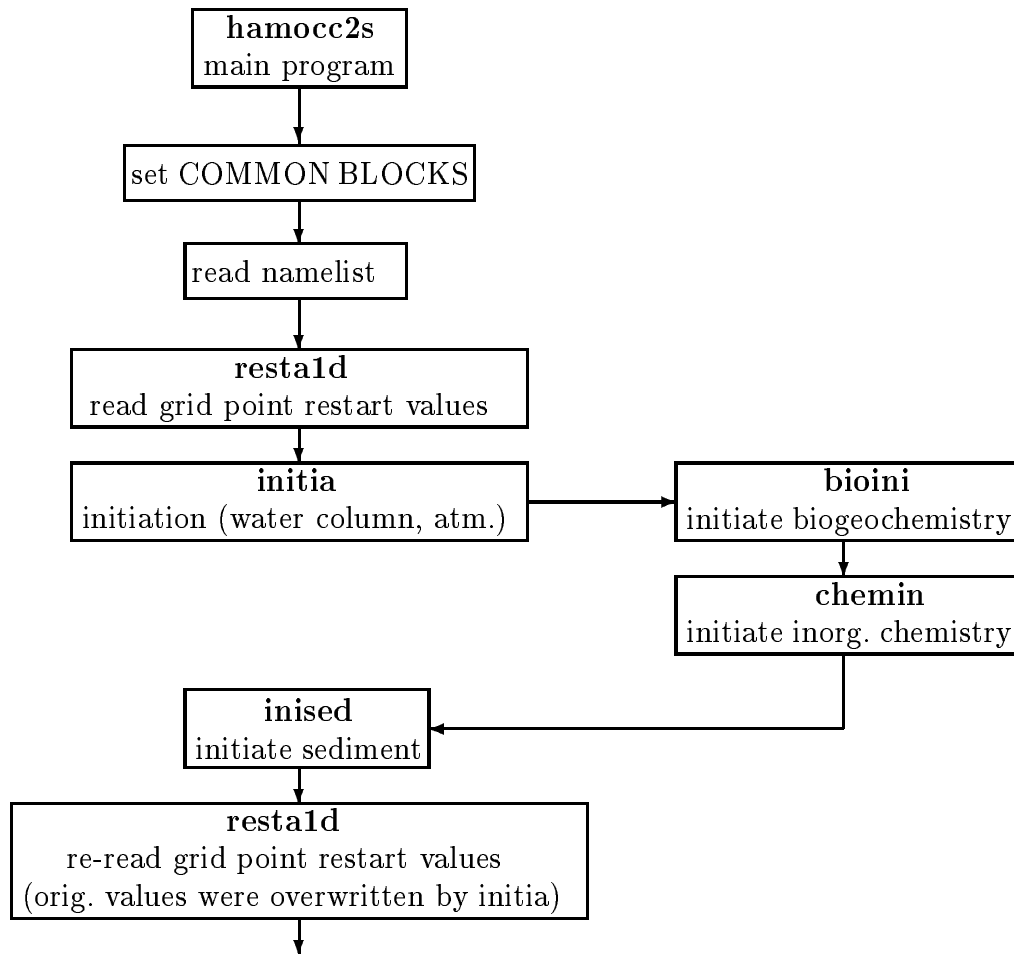
Flow chart for full 3-dimensional model:

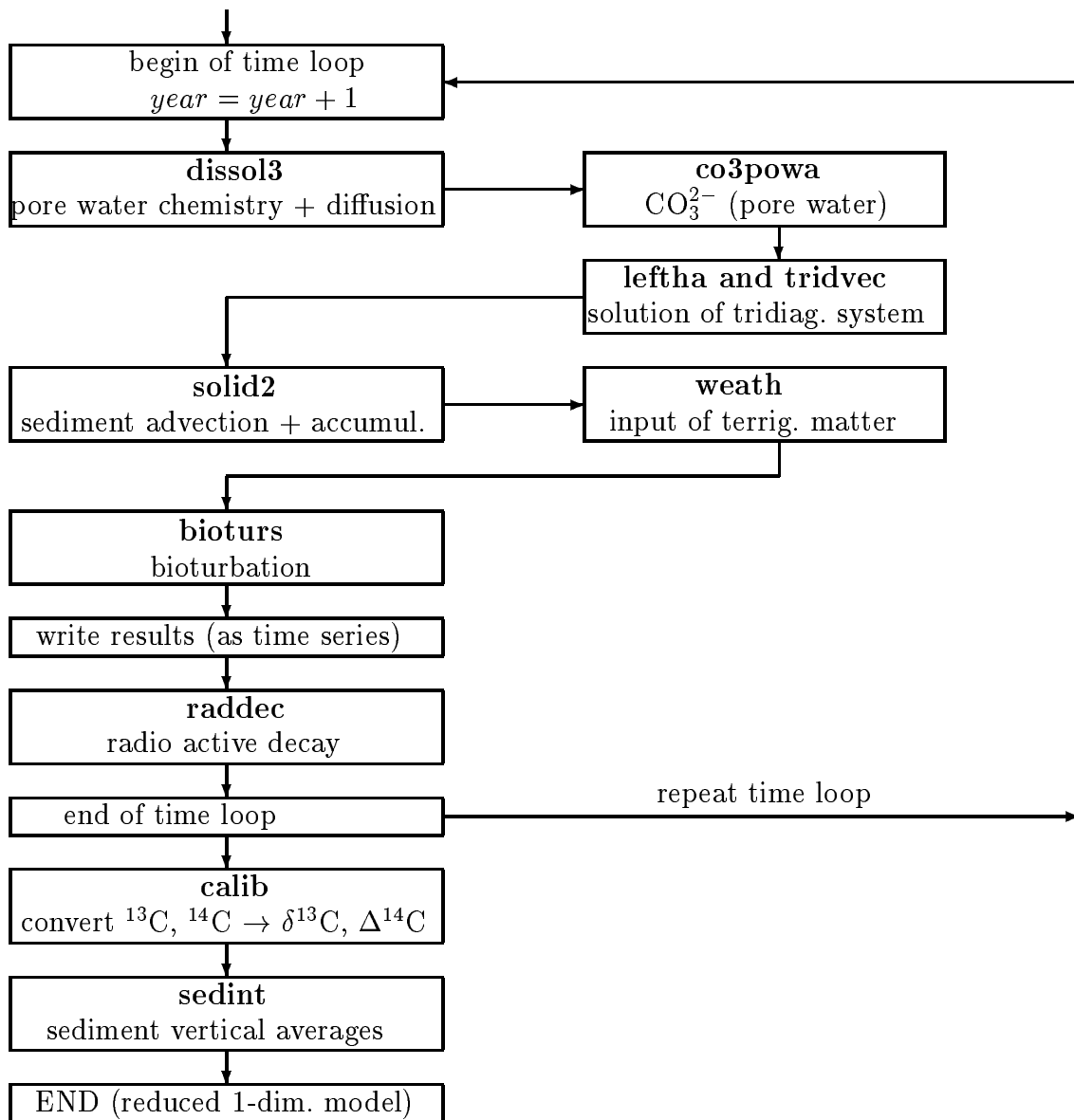






Flow chart for reduced 1-dimensional model:





4 USER'S GUIDE

All files necessary for a model run are summarised on:

schauer: /pool/modelle/hamocc2s/ha_694_1_pub_990910a.tar

The files are retrieved from the tar-file using the command:

tar -xvf ha_694_1_pub_990910a.tar .

The documented version is running on a Cray Unix system in batch mode. (It can, however, be run on any UNIX system, provided the binary files were converted to IEEE

or another readable format.) It has been proven very convenient to keep the shell script for running the model and the source code within one file. This is file:

ha_694_1

within ha_694_1_pub_990910a.tar. All COMMON blocks (.h-files), the main program (main.F) and all subroutines and functions (.F-files) are copied to single files on a temporary directory from ha_694_1. Thus it is easy, e.g., to change a variable name in the code of ha_694_1 without editing many small files.

4.1 HOW TO RUN THE MODEL – full 3-dimensional case

Here an abbreviated version of the shell script for the basic version is shown in Appendix A. On a Cray system this file is submitted by the “qsub” command.

Once you have the shell script file on disc, a model run is carried out as follows:

1. Specify in the shell script the directories where the program is executed, where the source code is compiled, and where the velocity file (output from LSG_OGCM) is found.
2. Fill in the namelist. Chose a small number for “intstp” (= the number of time steps to be carried out) in the beginning.
3. Adjust the makefile (compiler call, attributes ...) to your computer.
4. Submit the shell script (via “qsub ha_694_1” on a Cray system).
5. Wait until the job has finished.
6. Check the job-protocol (ha_6941.o...) and the program flow file “prot_694_1”. (Possibly correct errors and re-submit).
7. Plot/look at results.

The model can be run in different versions. These different versions are enabled/disabled by specifying special compiler options:

compiler option	number of layers in water col.	number of tracers in water col.	rare C- isotopes	velocity field file(s)	restart file
-D ke11	11	6	no	IFG0010M	R_694_00099911
-D ke11 -D nv6to10	11	switch 6/10	no/yes	IFG0010M	R_693_00069357
-D ke11 -D ciso	11	10	yes	IFG0010M	R_694_00099911

The standard version as on ha_694_1_pub_990910a.tar is prepared for a run without rare carbon isotopes. A restart file with ^{13}C and ^{14}C , however, is available. For a transition from a run without to a run with ^{13}C and ^{14}C if no appropriate restart file is available submit a short run with compiler option “-D ke11 -D nv6to10” using a double memory demand as for the basic model version. Then an extended restart file with the necessary array length for all tracers in the water column and the sediment is produced (where the rare C isotopes, of course, are not yet in equilibrium). This extended restart file can then

be used in a next step after recompiling the source code again with option “-D ke11 -D ciso”.

Also a - more time consuming - version with 22 layers in the water column (same sediment configuration as for 11-layer version) is available upon request. The source code is already prepared for the corresponding modifications (e.g., computation of explicit vertical diffusion coefficients from the local vertical in situ density difference). Option “ke11” has to be replaced by “ke22” and the respective velocity field has to be specified.

4.2 HOW TO RUN THE MODEL – reduced 1-dimensional case

So far the 1-dimensional model has only been tested for the basic case with 11 layers and 6 tracers in the water column (“-D ke11”). Use of the model in the reduced 1-dimensional mode requires two steps. First a special restart file must be produced from which all necessary input data for the reduced model can be read later on. This is done by carrying out a short run after recompilation with option “-D ke11 -D wrild”. Then, in the second step, a grid point must be specified, at which the model will be integrated (zonal and meridional indices `id1` and `jd1` in `namelist`), and the model has to be compiled once more with option “-D ke11 -D read”. So far only a time series of the respective sediment column results is written as output in the 1-dimensional version. Refined output has to be provided by the individual user.

4.3 VELOCITY FIELD FILES

The present basic 11-layer run has been produced by use of VELOCITY field IFG0010M (interglacial, modern climatology) of Winguth et al. (1996). Further velocity files (also for 22 layers) are available on request.

5 POSTPROCESSING/PLOTS

5.1 INTRODUCTION

In order to visualize the results a plot package is available, which provides maps (horizontal distributions) of all 2-dimensional and 3-dimensional variables, meridional as well as zonal cross sections of 3-dimensional water column tracer arrays, and grid point plots allowing a synoptic few on everything which is happening at one single grid point. These plots can be conveniently produced in an interactive mode on a workstation. This plot package is suitable for all scalar output arrays from the geochemical model and the LSG-OGCM or all other output from an E-grid model with equidistant grid point spacing with respect to longitude-degree and latitude-degree metric (e.g., also arrays from some HOPE-E-grid models).

Furthermore a small plot program is available to plot mean model and observed depth profiles (from the GEOSECS data set, version as archived by PACODF, SIO) in the water column for a quicklook on the model's behaviour.

All plot programs discussed here are based on the NCAR-Graphics system. It should be easily possible, however, to replace the respective plot commands in the source code by appropriate commands for another graphics software. It would be desirable, that people do not develop their own plot software for the model, but rather adjust the present package to their working environment and send us their converted routines so that other people benefit from conversions which already have been made.

5.2 USER'S GUIDE FOR THE POST PROCESSOR "HAMPL"

Use of this plot package requires several modules which have to be provided in part by the user and in part can be copied from the DKRZ file server.

5.2.1 FILES, WHICH MUST BE PROVIDED BY THE USER

The user must provide the following formatted ASCII files which are automatically produced by the annual mean model on ha_694_1 (or can be produced from any other model code by adding appropriate write statements as shown below):

- Files containing the data to be plotted (2- and 3-dimensional tracer distributions). For each variable a separate file is required. (These are the output files *_plotin from ha_694_1.) These files have to be written in the following format:

```
jl1=3
jle=je-2
c 2-dimensional array
  open(70,file='x2d_plotin',form='formatted',status='unknown')
  write(70,'(8(1x,e10.4))')((a2(i,j),i=1,ie),j=jl1,jle)
  close(70,status='keep')
c 3-dimensional array
  open(70,file='x3d_plotin',form='formatted',status='unknown')
  write(70,'(8(1x,e10.4))')(((a3(i,j,k),i=1,ie),j=jl1,jle),k=1,ke)
  close(70,status='keep')
```

- A depth and geometry information file containing the standard layer thicknesses at u- and w-points, the standard levels (u and w levels), the individual layer thicknesses at each box (3-dim. arrays, scalar and vector points), the bottom depths (2-dim. arrays, scalar and vector points), and the layer thicknesses of solid sediment. All numbers in the depth information file are given in m except for the layer thicknesses in the sediment which have to be provided in cm. The information on the sediment layer thickness may be missing as long as no maps of 3-dimensional sediment arrays or grid point plots are produced later on. (This is the output file `depthinfo` from `ha_694_1`.) This file has to be written in the following format:

```

jl1=3
jle=je-2
open(97,file='depthinfo',form='formatted',status='unknown')
c standard layer thickness u points
write(97,'(5(1x,e12.6))'dz
c standard layer thickness w points
write(97,'(5(1x,e12.6))'dzw
c standard level u points
write(97,'(5(1x,e12.6))')tiestu
c standard level w points
write(97,'(5(1x,e12.6))')tiestw
c individual layer thickness scalar points
write(97,'(5(1x,e12.6))')
* ((ddz(i,j,k),i=1,ie),j=jl1,jle),k=1,ke)
c individual layer thickness vector points
write(97,'(5(1x,e12.6))')
* ((ddu(i,j,k),i=1,ie),j=jl1,jle),k=1,ke)
c bottom depth scalar points
write(97,'(5(1x,e12.6))')
* ((deftp(i,j),i=1,ie),j=jl1,jle)
c bottom depth vector points
write(97,'(5(1x,e12.6))')
* ((deptu(i,j),i=1,ie),j=jl1,jle)
c layer thicknesses of solid sediment
c (this line may be missing if no sediment plots are made)
write(97,'(5(1x,f12.6))')(ddzs(ks),ks=2,kse)
close(97,status='keep')

```

- File with mean observed and modelled profiles (at identical positions). This is file “inventories” from the annually averaged model as described here. This file may be missing. You then cannot plot mean profiles, but the other plot types.

5.2.2 FILES, WHICH ARE PROVIDED BY DKRZ

The following files can be copied from the DKRZ file server (see below):

- Some depth and geometry information files which are already available:

file	originating from run
<code>depthinfo_11_ifg</code>	<code>ha_694_1</code> , 11 layers, run as described here, velocity field IFG0010M (Winguth et al., 1996)
<code>depthinfo_11_atos1</code>	velocity field ATOS1 of Maier-Reimer et al. (1993)
<code>depthinfo_15</code>	15 layers version, Maier-Reimer (1993)
<code>depthinfo_22</code>	22 layers version, as used in Heinze et al. (1998)
<code>depthinfo_22_emr</code>	22 layers version, June 1999, Maier-Reimer pers. comm.

- Examples for plot input files:
`alkali_plotin`, `alkas_plotin`, `cal12sf_plotin`, `cal13sf_plotin`, `cal12st_plotin`, `claysf_plotin`,
`clayst_plotin`, `co3_plotin`, `delta13c_plotin`, `opacfst_plotin`, `opalsf_plotin`, `opalst_plotin`,
`oxygen_plotin`, `oxygs_plotin`, `phosph_plotin`, `phosphs_plotin`, `poc12_plotin`, `poc12sf_plotin`,
`poc13sf_plotin`, `poc12st_plotin`, `prcaca_plotin`, `prorca_plotin`, `psili_plotin`, `sco12s_plotin`,
`sco13s_plotin`, `sco212_plotin`, `silica_plotin` and `silics_plotin`.

- Source code for plotting the data:
main.F colram.F datinp.F depinp.F dfclrs.F extmer.F extzon.F fildep.F fillev.F filmer.F filzon.F fil3d.F intlev.F obssecm.F openf.F openobs.F plaxes.F plcruis.F plgrmap.F plgrpoi.F plmap.F plmprof.F plsecm.F plsecz.F pltrack.F posfil.F position.F reverse.F setinp.F smoomap.F traind.F plus file parcom.h (COMMON-blocks and parameters) and the makefile.
- Specification file “sets” (different versions for 11, 15, and 22 layers).
- Position index files for meridional cross sections: secind_.*.
- Files containing data from observations (so far only the GEOSECS data) for a comparison with model results in meridional cross section plots:

filename	contents/purpose
stations_*	listings of stations with observations used for compiling the cruise tracks for single sections
*_geosecs_obs	GEOSECS data for single variables
secdat_geosecs_*. *	interpolated GEOSECS cross sections of observations (one file for each section and each variable)

5.2.3 HOW TO START

Select a machine where you want to produce the plots (preferably a UNIX workstation). NCAR-Graphics should be available (otherwise you have to modify the source text) as well as a previewer (here “idt” is used with subsequent transformation to a postscript file with “ctrans”.) Create a directory where you want to make the calculations.

5.2.4 HOW TO COPY THE FILES FROM THE DKRZ FILE SERVER

Go into the directory where you plan to make the plotting and type:

```
ftp schauer
(login)
cd /pool/modelle/hamocc2s
get hampl_pub_990910a.tar
(or get hampl_pub_short_990910a.tar if you are not interested in the observations)
by
tar -xvf hampl_990910a.tar
```

You should then have all the files described above on your disc.

5.2.5 HOW TO PRODUCE SOME EXAMPLE PLOTS

After having copied the files from the file server and unpacked everything you can produce some example plots (not yet with your own data). This procedure should work on the DKRZ Sun server “regen” using NCAR version 4.0 or 4.1.

The specification file “sets” is prepared for plotting a meridional phosphate cross section along the western Atlantic (see also Fig. 1 in Appendix B). Type “make” to be sure that the program is compiled. Then type “pl.x”. If everything works you should receive a file “gmeta”. You can preview it by typing “idt gmeta”. You should see the plot of Fig. 2 (Appendix B) on screen. Do NOT print gmeta directly. In order to print the plot you have to convert it to a postscript file by using “ctrans” with the script “g2ps” and you will get a file gmeta.psc which you can print by using “lpr -P... gmeta.psc”. The script “g2ps” contains the following command which you may modify to your needs:

```
ctrans -d ps.land.color -window 0.:0.:1.:1. gmeta > gmeta.psc
```

Alternatively you could view at gmeta.psc using “ghostview gmeta.psc”.

In a second example, a coloured map of organic carbon export production is created. Copy file sets_map onto sets (you could also edit the file “sets” according to Fig. 3, Appendix B; details about this are described further below). Again type “pl.x”. On “gmeta” you will receive the plot as shown in Fig. 4 (Appendix B), which again can be previewed through “idt gmeta” and printed via “g2ps” and “lpr -P... gmeta.psc”.

Further examples are described in the paragraphs addressing specific questions below.

5.2.6 HOW TO CHANGE THE HORIZONTAL DIMENSIONS

This package is prepared for plotting E-grid data on a 72×72 horizontal grid with geographical grid point positions as for the LSG-OGCM (version of Maier-Reimer et al. 1993). Potentially, the horizontal dimensions can be changed in file parcom.h, parameters ie and je (zonal and meridional dimensions). In this case, however, the program has to be recompiled and the section index files secind_* and all files for comparison with observations have to be provided in new versions. This has not been attempted yet.

5.2.7 HOW TO CHANGE THE NUMBER OF LAYERS

Currently, the LSG-OGCM and the carbon cycle/biogeochemical model are used with 11, 15, and 22 layers. The plot package as you copy it from the DKRZ file server is prepared for 11 layers. You can switch to another vertical resolution through the following steps:

- Change parameter ke in file parcom.h to the number of layers wanted.
- Recompile by typing “make”.
- Edit file “sets”:
 - Change the number of levels in the second row to the actual number (same as ke in file parcom.h).
 - Select the corresponding bottom topography file (e.g. “depthinfo_22” for 22 layers) by specifying 0=no and 1=yes. If you have created your own depthinfo-file copy this file into the plot directory (or any other directory) and specify its name (and path) in “sets” (e.g. by changing “depthinfo_11_atos1” into “my-depthfile” and switching it on through replacing 0 by 1 in the first column of the respective row)

- Adjust the number of lines below “which level ?” to the actual number of levels, so that you can switch on/off all levels for map plots.
- Copy your own data into the plot directory, specify the file names in “sets” (see below “How to specify from which file(s) data shall be plotted”) and type “plx”.

5.2.8 HOW TO CHANGE THE TOPOGRAPHY/DEPTH INFORMATION FILE

- Select the corresponding bottom topography file in file “sets” (e.g. “depthinfo_22” for 22 layers) by specifying 0=no and 1=yes. If you have created your own depthinfo-file, copy this file into the plot directory (or any other directory) and specify its name (and additionally the full path to it, if necessary) in “sets” (e.g. by changing “depthinfo_11_atos1” into “my-depthfile” and switching it on through replacing 0 by 1 in the first column of the respective row)
- Change the number of levels in the second line of file “sets” to the actual number.
- If the number of levels changes with respect to a previous run follow the procedure as described above under “How to change the number of layers”.

5.2.9 HOW TO SPECIFY FROM WHICH FILE(S) DATA SHALL BE PLOTTED

After you have copied your own model results (for formats see “Files, which must be provided by the user” above) into the directory, where the plots are produced, specify the file name on the very right column of file “sets” in the row of the respective variable to be plotted (e.g., if your phosphate data are on file “PO4own” replace “phosph_plotin” in file “sets”, see Fig. 1, by “PO4own”). You need not specify whether your input data contain a 2- or 3-dimensional data set. The program identifies this by itself. See also paragraphs, “How to add new variables to the post processor”.

5.2.10 HOW TO SMOOTH DATA BEFORE CONTOURING THEM

Smoothing can be applied to maps and sections. The smoothing is done directly before contouring the data (in subroutine smoomap.F for maps, and within subroutines plsecm.F and plsecz.F for sections). You can specify the degree of smoothing in line number 9 of file “sets”. Specifying “0” will result in no smoothing at all. Specifying “10” will result in strong smoothing. Usually “1” should be sufficient for model data.

5.2.11 HOW TO SWITCH BETWEEN COLOURED AND BLACK&WHITE PLOTS

During one plot run either coloured or b&w plots are produced. You specify this in line 15 of file “sets” (0=b&w, 1=colours). For coloured plots the number of contour lines (to be specified in each row for each variable in file “sets”) must be 13 (15 colours are available). For b&w plots the number of contour lines can be chosen arbitrarily up to 99.

5.2.12 HOW TO CHANGE THE COLOUR OF CONTINENTS/BOTTOM TOPOGRAPHY

If you set “1” in the first column in line 16 of file “sets”, continents/land points are filled with black (see Figs. 1 and 2). If you set “0”, they are kept white (see Figs. 3 and 4).

5.2.13 HOW TO WRITE AN INDIVIDUAL COMMENT ON THE PLOT

You can specify the three text strings “string1”, “string2”, and “string3” in file “sets” according to your needs (they may be left blank).

5.2.14 HOW TO SPECIFY THE TYPE OF PLOT

This is specified in the first column of file “sets” below “which type of plot?”. You have the choice of maps (“levelplots”, in the water column or the sediment), meridional sections, and zonal sections.

These plots can be drawn easily from various configurations of the Hamburg biogeochemical model. Furthermore, mean profile plots (at GEOSECS data points), maps of single levels within the bioturbated sediment, and synoptic water column/sediment plots for single grid points can be directly produced from the output which is provided by the annually averaged model as described here (other model configurations would have to be modified for producing the respective output, which generally should be easily possible).

More than one type may be specified at once. An exception are maps of single sediment layers, which can only be plotted in a run where all other plot types are disabled (because of the different depth structure as compared to the water column).

5.2.15 HOW TO SPECIFY THE LEVELS TO BE PLOTTED

At first you have to set “1: levelplot” in file “sets”. The depth level to be plotted is specified in the first column of file “sets” below “which level?”. More than one level can be switched on. For 2-dimensional arrays, the choice of the level does not matter.

5.2.16 HOW TO PLOT SINGLE LAYERS OF A 3-D SEDIMENT FILE

You have to set “1: levelplot in sediment” and to specify the specific depth levels within the bioturbated sediment zone below “Y/N index of level in sediment” in file “sets”. If you have enabled “1: levelplot in sediment” no other plot type can be produced within the same run (due to the different dimensions of the input data arrays for sediment and water column plots). An example for the configuration file “sets” and the resulting plot are given in Figs. 5 and 6.

5.2.17 HOW TO PLOT COLOURED PIXEL MAPS

You have to set “1: levelplot” and additionally “1: levelplot pixel” in file “sets”. Further specify the levels to be plotted. You will get mosaic like pictures where each grid point is coloured. No contouring is performed. Smoothing is automatically disabled. Pixel plot maps are the choice for plotting horizontal arrays which have gaps due to undefined grid points such as observed data of sediment components (e.g., opal weight percentages). The map of Fig. 4 plotted as a pixel map is shown in Fig. 7.

5.2.18 HOW TO SPECIFY THE MERIDIONAL CROSS SECTION TO BE PLOTTED

At first you have to set “1: meridional section” in file “sets”. The meridional cross section to be plotted is specified below “which meridional section ?” in file “sets” (0=no, 1=yes). In each row for each station you find a character string identifying the section and a file name containing the zonal indices for the respective section. You can create your own cross sections by keeping the same format as files `secind_*`. E.g., if you have produced your own western Atlantic section on file “secind_own”, replace the name string “Western Atlantic GEOSECS” by “Western Atlantic own ” and the file name “secind_geosecs_watl” by “secind_own”.

5.2.19 HOW TO SPECIFY THE ZONAL CROSS SECTION TO BE PLOTTED

At first you have to set “1: zonal section” in file “sets”. Then specify the zonal section below “which zonal section ?” in “sets”. You can create your own zonal section by modifying the meridional index (“j=...”) at the righthand side of each zonal section specification row. An example for the configuration file “sets” and the resulting plot for a zonal silicic acid cross section near the equator are given in Figs. 8 and 9.

5.2.20 HOW TO PLOT MEAN PROFILES

Mean profiles of model results and observations from the GEOSECS program can be plotted by providing an input file “inventories” (output from the annually averaged model), which already contains the profiles. The compilation of the mean profiles is not carried out within the post processor. In order to plot the mean profiles, enable “1: mean profiles (water column)” below “which type of plot ?” in file “sets”. An example for the resulting plot is given in Fig. 10.

5.2.21 HOW TO PRODUCE SINGLE GRID POINT PLOTS

The following files must be available for producing synoptic views on several water column and sediment variables at single grid points (the $\delta^{13}\text{C}$ files may be missing, for formats see “Files, which must be provided by the user” above):

file name	variable
sco212_plotin	C_T (DIC) (water column)
alkali_plotin	alkalinity (water column)
phosph_plotin	dissolved phosphate (water column)
oxygen_plotin	dissolved oxygen (water column)
silica_plotin	silicic acid (water column)
delta13c_plotin	$\delta^{13}\text{C}$ (water column)
sco12s_plotin	C_T (pore water)
alkas_plotin	alkalinity (pore water)
phosphs_plotin	dissolved phosphate (pore water)
oxygs_plotin	dissolved oxygen (pore water)
silics_plotin	silicic acid (pore water)
sco13s_plotin	$\delta^{13}\text{C}$ (pore water)
cal12sf_plotin	CaCO_3 sediment
cal13sf_plotin	$\delta^{13}\text{C}$ of CaCO_3 sediment
poc12sf_plotin	organic carbon sediment
poc13sf_plotin	$\delta^{13}\text{C}$ of organic carbon sediment
opalsf_plotin	opal sediment
claysf_plotin	clay sediment (inert component)

In order to produce grid point plots modify file “sets”:

- Enable “1: single grid point plot” below “which type of plot ?”.
- Specify which grid point(s) have to be plotted below “which grid point ?”. You can either specify explicitly the zonal and meridional indices (refer to Fig. 21). If you set i and j to 0, alternatively a given latitude and longitude can be specified and the grid point indices of the nearest grid point position are computed later on. Under “name” you can define a string which will be written on the respective plot.

You will receive a map indicating the grid points which you have chosen and the respective grid point plots. Please refer to Figs. 11, 12, 13 for examples concerning the configuration file “sets”, the orientation map, and the single grid point plot for a position in the North Atlantic Ocean.

5.2.22 HOW TO SPECIFY WHICH VARIABLE(s) SHALL BE PLOTTED

Set for each variable that shall be plotted in the leftmost column of file “sets” below the string “which variable ?” a “1”. You can specify several parameters simultaneously.

5.2.23 HOW TO SPECIFY NUMBER AND INTERVAL OF CONTOUR LINES

For each variable to be plotted you have one row in file “sets” (below the string “which variable?”) where the contour line information is set. The number of contour lines is set automatically to 13 in case of colour plots (15 colours available), for b&w-plots you

can choose up to 99 lines. Further you can specify the minimum of contour lines and the contour interval.

In special cases non-eqidistant contour intervals can be selected. Set the number of contour lines for the respective variable to 0. In this case the values of contour lines to be drawn are read from a file “special_lines” in which you have to explicitly specify the contour values (one value per line, leftbound). You can specify up to 99 lines. In case of colour plots only the first 13 values are used.

5.2.24 HOW TO CHANGE THE NAME OF THE VARIABLE ON THE PLOT

You can change the name of a variable (including the associated unit) in the row for each variable to be plotted below the string “which variable?” in file “sets”. It is this character string which is plotted on top of the respective diagram. Also if you change the units in your plot-input data you can adjust this character string to the actual units used.

5.2.25 HOW TO ADD NEW VARIABLES TO THE POST PROCESSOR

You can easily introduce a new variable to the post processor. First copy your new data into the directory where the plot is produced. Then chose any row below “which variable ?” in file “sets” and change it to your needs. Specify from left to right, that the parameter shall be plotted (change “0” to “1”), fill in a character string for name and physical/chemical units of the variable, select number of contour lines and contour interval, specify whether this variable is defined at scalar or vector point positions (plots of variables at vector point positions are not yet available), and finally fill in the name of your new file with the data to be plotted at the right hand side of the row. You may also arbitrarily exchange the sequence of different rows, with one exception: the 9th row is reserved for the CO_3^{2-} concentration, because a diagnostic CaCO_3 lysocline (after Broecker and Takahashi, 1978) is plotted into the respective sections. If you want to plot observed data see paragraph “How to compare model data with observations” below. In the example configuration up to 40 different variables can be specified. If you change the number of total possible variables (i.e., the number of “variable rows” in file “sets” below “which variable ?” you have to adjust the parameter “npar=...” in file parcom.h accordingly).

5.2.26 HOW TO COMPARE MODEL DATA WITH OBSERVATIONS

So far only observed data from the GEOSECS program and only meridional cross sections are considered. This plot package provides the possibility to produce diagrams of observed and modelled tracer distributions with identical contour lines and aspect ratio and also to produce difference plots of modelled minus observed values. For coupling to the observed data the rows for variables MUST be in a certain the sequence (with pot. temperature being the first “variable row”) in file “sets” (see also to Fig. 1):

row 1 potential temperature
row 2 salinity
row 3 C_T
row 4 A_T
row 5 dissolved phosphate
row 6 dissolved oxygen
row 7 POC
row 8 silicic acid
row 9 carbonate ion concentration
row 10 delta C-13 of C_T
row 11 Delta C-14 of C_T

As different stations from the GEOSECS expeditions cover different sets of variables, for each variable and each section, a special section index file is necessary which contains the information of the zonal index in the plot array for a given meridional index. Especially, sometimes a more “wiggly” cruise track must be chosen for variables with a comparatively poor data coverage. For each cross section and each variable a different secind.* file has to be specified explicitly by the user on the right hand side of each “section row” below “which meridional section ?” in file “sets”. This is not done automatically, because for routine plots, usually it is desirable to plot each variable along exactly the same cruise track.

Observed cross sections are available for the following variables and sections:

variable	merid. cross section	observed data file	section index file
potential temperature	Western Atlantic GEOSECS	secdat_geosecs_watl_tem	secind_geosecs_watl_tem
potential temperature	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_tem	secind_geosecs_eatl_tem
potential temperature	Western Pacific GEOSECS	secdat_geosecs_wpac_tem	secind_geosecs_wpac_tem
potential temperature	Eastern Pacific GEOSECS	secdat_geosecs_epac_tem	secind_geosecs_epac_tem
potential temperature	Western Indian Ocean GEOSECS	secdat_geosecs_wind_tem	secind_geosecs_wind_tem
potential temperature	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_tem	secind_geosecs_eind_tem
potential temperature	Central Indian Ocean GEOSECS	secdat_geosecs_cind_tem	secind_geosecs_cind_tem
salinity	Western Atlantic GEOSECS	secdat_geosecs_watl_sal	secind_geosecs_watl_sal
salinity	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_sal	secind_geosecs_eatl_sal
salinity	Western Pacific GEOSECS	secdat_geosecs_wpac_sal	secind_geosecs_wpac_sal
salinity	Eastern Pacific GEOSECS	secdat_geosecs_epac_sal	secind_geosecs_epac_sal
salinity	Western Indian Ocean GEOSECS	secdat_geosecs_wind_sal	secind_geosecs_wind_sal
salinity	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_sal	secind_geosecs_eind_sal
salinity	Central Indian Ocean GEOSECS	secdat_geosecs_cind_sal	secind_geosecs_cind_sal
C_T	Western Atlantic GEOSECS	secdat_geosecs_watl_tco2	secind_geosecs_watl_tco2
C_T	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_tco2	secind_geosecs_eatl_tco2
C_T	Western Pacific GEOSECS	secdat_geosecs_wpac_tco2	secind_geosecs_wpac_tco2
C_T	Eastern Pacific GEOSECS	secdat_geosecs_epac_tco2	secind_geosecs_epac_tco2
C_T	Western Indian Ocean GEOSECS	secdat_geosecs_wind_tco2	secind_geosecs_wind_tco2
C_T	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_tco2	secind_geosecs_eind_tco2
C_T	Central Indian Ocean GEOSECS	secdat_geosecs_cind_tco2	secind_geosecs_cind_tco2
A_T	Western Atlantic GEOSECS	secdat_geosecs_watl_alk	secind_geosecs_watl_alk
A_T	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_alk	secind_geosecs_eatl_alk
A_T	Western Pacific GEOSECS	secdat_geosecs_wpac_alk	secind_geosecs_wpac_alk
A_T	Eastern Pacific GEOSECS	secdat_geosecs_epac_alk	secind_geosecs_epac_alk
A_T	Western Indian Ocean GEOSECS	secdat_geosecs_wind_alk	secind_geosecs_wind_alk
A_T	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_alk	secind_geosecs_eind_alk
A_T	Central Indian Ocean GEOSECS	secdat_geosecs_cind_alk	secind_geosecs_cind_alk
dissolved phosphate	Western Atlantic GEOSECS	secdat_geosecs_watl_po4	secind_geosecs_watl_po4
dissolved phosphate	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_po4	secind_geosecs_eatl_po4
dissolved phosphate	Western Pacific GEOSECS	secdat_geosecs_wpac_po4	secind_geosecs_wpac_po4
dissolved phosphate	Eastern Pacific GEOSECS	secdat_geosecs_epac_po4	secind_geosecs_epac_po4
dissolved phosphate	Western Indian Ocean GEOSECS	secdat_geosecs_wind_po4	secind_geosecs_wind_po4
dissolved phosphate	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_po4	secind_geosecs_eind_po4
dissolved phosphate	Central Indian Ocean GEOSECS	secdat_geosecs_cind_po4	secind_geosecs_cind_po4

(continued on next page)

(continued) variable	merid. cross section	observed data file	section index file
dissolved oxygen	Western Atlantic GEOSECS	secdat_geosecs_watl_o2	secind_geosecs_watl_o2
dissolved oxygen	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_o2	secind_geosecs_eatl_o2
dissolved oxygen	Western Pacific GEOSECS	secdat_geosecs_wpac_o2	secind_geosecs_wpac_o2
dissolved oxygen	Eastern Pacific GEOSECS	secdat_geosecs_epac_o2	secind_geosecs_epac_o2
dissolved oxygen	Western Indian Ocean GEOSECS	secdat_geosecs_wind_o2	secind_geosecs_wind_o2
dissolved oxygen	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_o2	secind_geosecs_eind_o2
dissolved oxygen	Central Indian Ocean GEOSECS	secdat_geosecs_cind_o2	secind_geosecs_cind_o2
silicic acid	Western Atlantic GEOSECS	secdat_geosecs_watl_sil	secind_geosecs_watl_sil
silicic acid	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_sil	secind_geosecs_eatl_sil
silicic acid	Western Pacific GEOSECS	secdat_geosecs_wpac_sil	secind_geosecs_wpac_sil
silicic acid	Eastern Pacific GEOSECS	secdat_geosecs_epac_sil	secind_geosecs_epac_sil
silicic acid	Western Indian Ocean GEOSECS	secdat_geosecs_wind_sil	secind_geosecs_wind_sil
silicic acid	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_sil	secind_geosecs_eind_sil
silicic acid	Central Indian Ocean GEOSECS	secdat_geosecs_cind_sil	secind_geosecs_cind_sil
CO ₂ ⁻	Western Atlantic GEOSECS	secdat_geosecs_watl_co3	secind_geosecs_watl_co3
CO ₂ ⁻	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_co3	secind_geosecs_eatl_co3
CO ₂ ⁻	Western Pacific GEOSECS	secdat_geosecs_wpac_co3	secind_geosecs_wpac_co3
CO ₂ ⁻	Eastern Pacific GEOSECS	secdat_geosecs_epac_co3	secind_geosecs_epac_co3
CO ₂ ⁻	Western Indian Ocean GEOSECS	secdat_geosecs_wind_co3	secind_geosecs_wind_co3
CO ₂ ⁻	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_co3	secind_geosecs_eind_co3
CO ₂ ⁻	Central Indian Ocean GEOSECS	secdat_geosecs_cind_co3	secind_geosecs_cind_co3
$\delta^{13}\text{C}$ of C_T	Western Atlantic GEOSECS	secdat_geosecs_watl_d13c	secind_geosecs_watl_d13c
$\delta^{13}\text{C}$ of C_T	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_d13c	secind_geosecs_eatl_d13c
$\delta^{13}\text{C}$ of C_T	Western Pacific GEOSECS	secdat_geosecs_wpac_d13c	secind_geosecs_wpac_d13c
$\delta^{13}\text{C}$ of C_T	Eastern Pacific GEOSECS	secdat_geosecs_epac_d13c	secind_geosecs_epac_d13c
$\delta^{13}\text{C}$ of C_T	Western Indian Ocean GEOSECS	secdat_geosecs_wind_d13c	secind_geosecs_wind_d13c
$\delta^{13}\text{C}$ of C_T	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_d13c	secind_geosecs_eind_d13c
$\delta^{13}\text{C}$ of C_T	Central Indian Ocean GEOSECS	secdat_geosecs_cind_d13c	secind_geosecs_cind_d13c
$\Delta^{14}\text{C}$ of C_T	Western Atlantic GEOSECS	secdat_geosecs_watl_D14c	secind_geosecs_watl_D14c
$\Delta^{14}\text{C}$ of C_T	Eastern Atlantic GEOSECS	secdat_geosecs_eatl_D14c	secind_geosecs_eatl_D14c
$\Delta^{14}\text{C}$ of C_T	Western Pacific GEOSECS	secdat_geosecs_wpac_D14c	secind_geosecs_wpac_D14c
$\Delta^{14}\text{C}$ of C_T	Eastern Pacific GEOSECS	secdat_geosecs_epac_D14c	secind_geosecs_epac_D14c
$\Delta^{14}\text{C}$ of C_T	Western Indian Ocean GEOSECS	secdat_geosecs_wind_D14c	secind_geosecs_wind_D14c
$\Delta^{14}\text{C}$ of C_T	Eastern Indian Ocean GEOSECS	secdat_geosecs_eind_D14c	secind_geosecs_eind_D14c
$\Delta^{14}\text{C}$ of C_T	Central Indian Ocean GEOSECS	secdat_geosecs_cind_D14c	secind_geosecs_cind_D14c

If you want to plot an observed section specify “1: plot observed” in file “sets” after having set “1: meridional section” the rest of the procedure being the same as for plotting usual meridional cross sections.

If you want to plot model minus observations differences specify “1: plot mod-obs” in file “sets” after having set “1: meridional section” the rest of the procedure again being the same as for plotting usual meridional cross sections. An appropriate readjustment of the contour line minimum is carried out automatically.

5.2.27 HOW THE OBSERVED SECTION DATA ARE COMPILED

It is not recommended to do this if the user is unexperienced with the plot package.

At first you need a set of station positions where observations are available. These stations are combined to meridional cross section later on. These positions have to be provided by the user. Positions must be written in the following format to the position file which is called “cruise_track”:

```
write(iunit,'(9x,2(1x,f8.3))')rlatit,rlongit
```

An example for such a file is given in Fig. 14. This example was taken from the construction of the western Pacific GEOSECS section for dissolved phosphate. In order to check the cruise track (also for editing until the correct amount and configuration of stations are available) a map plot can be produced by running “pl.x” after setting “1: cruise track

check only” after “1: levelplot” in file “sets” (example in Fig. 15).

In a next step a meridional cross section is constructed from the station positions as given in file “cruise_track”. To each position the next available point of the regular grid with model informations as derived from the original E-grid is determined. (The regular grid is the original scalar array with interpolated model values also at vector point positions.) The corresponding station position is approximated by the position of this respective nearest position of the regular grid. If longitude bands are not covered by an observed station, a grid position (in the regular grid) is determined onto which information from the nearest neighbouring grid points containing information of observations will be interpolated later on. This new cruise track on the regular grid will be constructed if, after “1: levelplot” , “1: cruise track check only” and additionally “1: fill meridional section” are set. After typing “pl.x” the resulting section indices are written to “secind_new” (with information whether information of observations is locally available) and a plot is produced indicating the original stations and the newly constructed cross section (see Figs. 16 and 17).

In the next step the observed data are interpolated and plotted along the given cross section as prescribed in file “secind_new”. At first, all level plot options are set to “0” in file “sets”. Then meridional cross sections are enabled by specifying “1: meridional section” and additionally “1: compile observed section”. The latter option forces interpolation of the observed station data. Below “which meridional section ?” enable, for example, “Western Pacific GEOSECS” and replace the section index file name “secind_geosecs_wpac” by “secind_new”. Again run “pl.x”. The data from stations listed in file “cruise_track” are then interpolated onto the regular plot grid using the same topography as the model (the topography is also interpolated on a regular grid from the original scalar E-grid configuration). If more than one observed datum from one station and one depth is encountered, these data are averaged. Result from this step is a data set on the plot grid (ready for contouring) written to a file. In our example this file is “secind_geosecs_wpac_po4”. The corresponding file names for each parameter and sections are set in subroutine openobs.F.

Problems can arise if the observed data array is too sparse. The interpolation method can be overridden by hand in subroutine obssecm.F. Important parameters are especially the maximum allowable vertical distance between two samples at one station and the zeroing of vertical weighting in cases that the lowermost sample is too far above the ocean floor.

If you add other sections than that listed in file “sets” (see Fig. 1) do the following:

- Enter a new line in file “sets” below “which meridional section ?” which specifies the new cross section according to your needs.
- Adjust the number of possible meridional cross sections in file parcom.h (parameter “nmsec=...”).
- Edit subroutine “openobs.F”: add the file name for the new section and each variable.
- Recompile by typing “make” and run again by “pl.x”.

You can plot the observed sections easily without producing the interpolated data array

each time newly, by enabling “1: meridional section” and “1: plot observed” and disabling “0: compile observed section ” in file “sets”. Also smoothing to various degrees can applied at this stage for individual plots from the same data array. For our example of phosphate along the western Pacific the corresponding plot of observed data is given in Fig. 18. The corresponding model section is plotted by disabling “0: plot observed” (see example plot in Fig. 19). Finally the difference modelled minus observed data is plotted through enabling “1: meridional section” and “1: plot mod-obs” in file “sets” (see example in Fig. 20). In the plots of the observed data and the model–observation differences the points where original data are available for interpolation are indicated by small dots.

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8 Appendix A: EXAMPLE OF A SHELL SCRIPT FOR RUNNING THE MODEL

This script is suitable for batch mode on a Cray system:

```
# QSUB-lt 900      # time limit
# QSUB-lm 8Mw      # memory limit
# QSUB-eo          # standard error and output
# QSUB-r ha_6941   # process-name
# QSUB
#
set -v
#
CRAYPROGDIR=yourdirectory/sources
CRAYRUNDIR=yourdirectory
LSGFILE=yourvelocitydirectory
cd $TMPDIR
# sources
#-----
cat > com_block.h << EOFcom_block
#ifdef readl
    parameter(ie=5,je=5,jl1=3,jle=3)
#else
    parameter(ie=72,je=76,jl1=3,jle=74)
#endif
#ifdef ciso
    parameter(ke=11,kep=ke+1,ieje=ie*je,nv=10,
etc. etc. ...
---
---
EOFcom_block
cat > com_sed.h << EOFcom_sed
---
---
cEOFcom_sed
cat > com_v12mnmt.h << EOFcom_v12mnmt
---
---
#endif
EOFcom_v12mnmt
cat > main.F << EOFmain
    program hamocc2s
---
---
    stop 'normal'
end
EOFmain
cat > advect.F << EOFadvect
    subroutine advect
---
---
    return
end
EOFadvect
cat > atmdif.F << EOFatmdif
    subroutine atmdif
---
---
    return
end
EOFatmdif
cat > bilanz.F << EOFbilanz
    subroutine bilanz
---
---
other subroutines and functions until...
---
EOFweath
ls -l
#
# copy files into directory for compilation
#-----
cp com_block.h $CRAYPROGDIR
cp com_v12mnmt.h $CRAYPROGDIR
cp com_sed.h $CRAYPROGDIR
cp main.F $CRAYPROGDIR
```

```

cp advect.F $CRAYPROGDIR
cp atmdif.F $CRAYPROGDIR
cp bilanz.F $CRAYPROGDIR
---
---
---
cp weath.F $CRAYPROGDIR
#
# makefile, compilation is done in the source code directory
#-----
cat > makefile <<'EOF1'
F90 = f90
FFLAGS = -m 1 -r 3
SAVBIN = -c
LIBFLAGS =
DEFLIST = -D ke11
OBSJ = main.o advect.o atmdif.o bilanz.o bioini.o biopro.o bioturs.o calib.o chemin.o co3powa.o co3waco.o dissol3.o
a.o modobs.o mosoli.o mowaco.o mowaf1.o outwri.o oxycon.o pools.o positio.o raddec.o reacir.o resta1d.o rho.o sedi
rfch.o tinsit.o tridia.o updrai.o weath.o
HEADERS1 = com_block.h com_v12mmt.h
HEADERS2 = com_block.h com_v12mmt.h com_sed.h

hamocc.x: ${OBSJ}
    ${F90} ${FFLAGS} ${LIBFLAGS} -o hamocc.x ${OBSJ}

main.o :    main.F ${HEADERS2}
    ${F90} ${FFLAGS} ${DEFLIST} ${SAVBIN} main.F
advect.o :  advect.F ${HEADERS1}
    ${F90} ${FFLAGS} ${DEFLIST} ${SAVBIN} advect.F
atmdif.o :  atmdif.F ${HEADERS1}
    ${F90} ${FFLAGS} ${DEFLIST} ${SAVBIN} atmdif.F
bilanz.o :  bilanz.F ${HEADERS2}
    ${F90} ${FFLAGS} ${DEFLIST} ${SAVBIN} bilanz.F
---
---
---
weath.o :  weath.F ${HEADERS2}
    ${F90} ${FFLAGS} ${DEFLIST} ${SAVBIN} weath.F
EOF1
cp makefile $CRAYPROGDIR
#
# jump to directory where source code is handled, compile program
#-----
cd $CRAYPROGDIR
rm hamocc.x
make
#
# program listing after compilation
#-----
pg $CRAYPROGDIR/main.lst
pg $CRAYPROGDIR/advect.lst
pg $CRAYPROGDIR/atmdif.lst
pg $CRAYPROGDIR/bilanz.lst
---
---
---
pg $CRAYPROGDIR/weath.lst
#
# jump to directory where model integration is carried out
#-----
cd $CRAYRUNDIR
#
# save integration protocol (standard output) from previous run
#-----
cp prot_694_1 prot_694_0
#
# fetch velocity filed file
#-----
cp $LSGFILE VELOCI
#
# save mean profiles from previous runs
#-----
cp inventories_old inventories_veryold
cp inventories inventories_old
#
# execute program, pipe standard out put to prot_...-file,
# stop if error, specify namelist
#-----
rm hamocc.x
cp $CRAYPROGDIR/hamocc.x .
chmod 700 hamocc.x
ls -l
set -e
ja
hamocc.x > prot_694_1 <<EOR
&setrun intstp=5
        timax=13700.
        runid='hamocc2_694

```

```

        ifulbi=0
        iyear0=0
        nyear0=0
        irstart=1
        iinvad=0
        isedini=0
        conc0=1.E-5
        cosi0=8.2E-9
        pendeo=77000.
        pendec=200000.
        pendes=1000000.
        caco3r=0.31
        calthre=0.7
        dustflu=1.0
        sisat=800.e-6
        rcorg=50.
        rccal=75.
        rcopal=50.
        sublth=0.5
        biotdb=15.
        id1=68
        jd1=35
        slc12p=21.68798966258214
        slc13p=21.68798966258214
        slc14p=21.68798966258214
        slalkp=32.69726875587821
        slpo4p=5.01077957481877
        slopalp=11.92964645954709
    &end
EOR
ja -st
set +e
ls -l
exit
# end of shell script

```

9 Appendix B: PLOT EXAMPLES

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Here you
can write
any text you want.

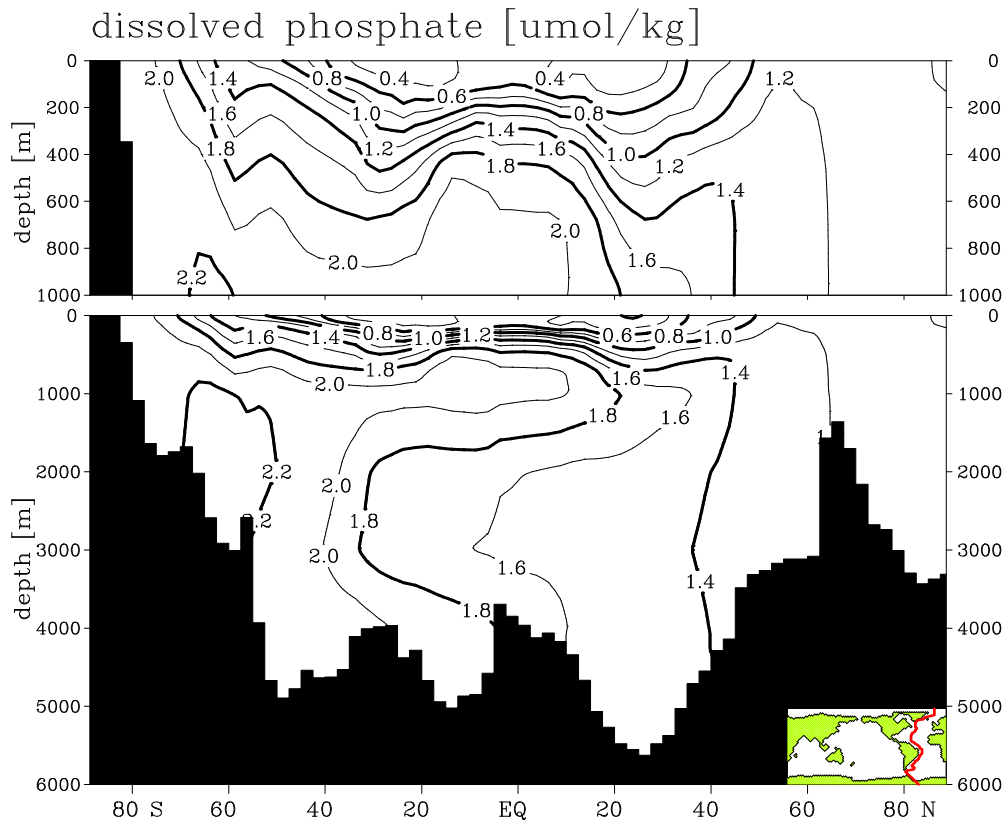


Figure 2: Resulting cross section with specifications from file “sets” as given in Fig. 1.

Here again you
can write
any text you want.

POC export production [gC/(m**2 yr)]

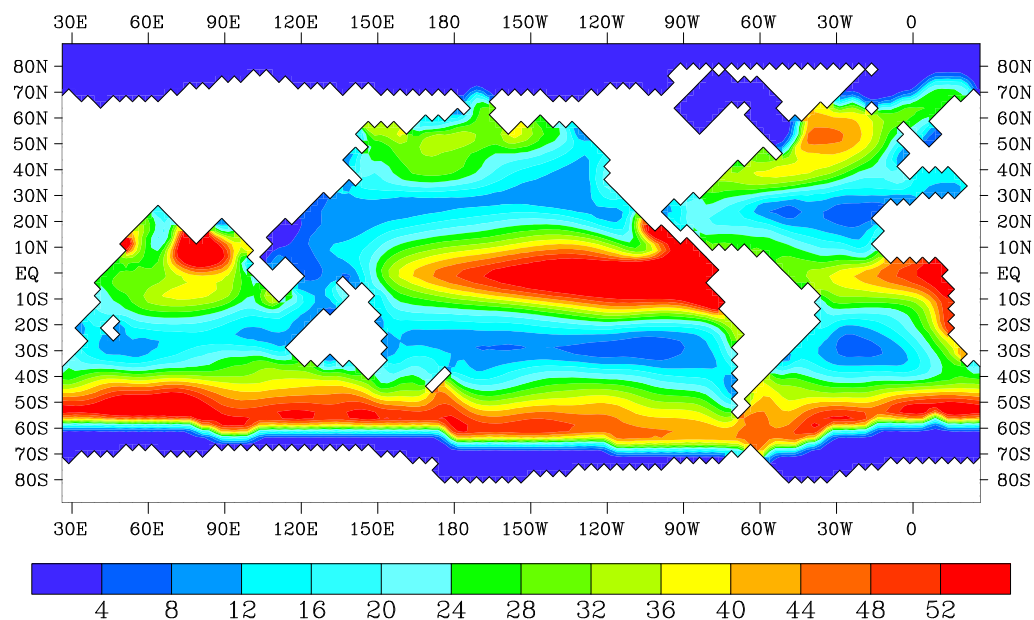


Figure 4: Resulting map with specifications from file “sets” as given in Fig. 3.

Figure 5: Example of file “sets” with selections for a plot of silicic acid in single layer within the sediment pore water.

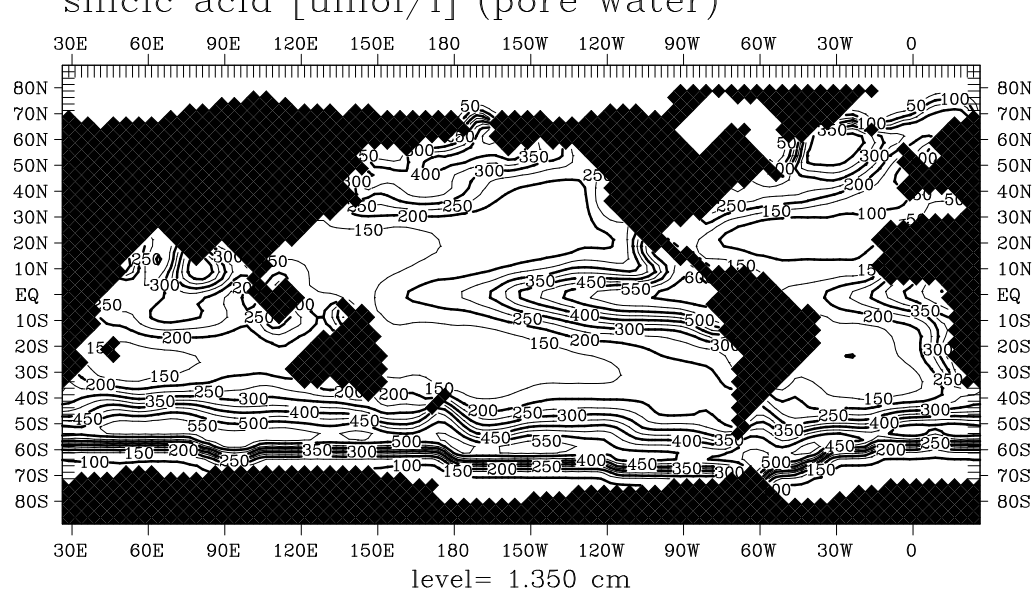


Figure 6: Resulting map within the bioturbated sediment with specifications from file “sets” as given in Fig. 5.

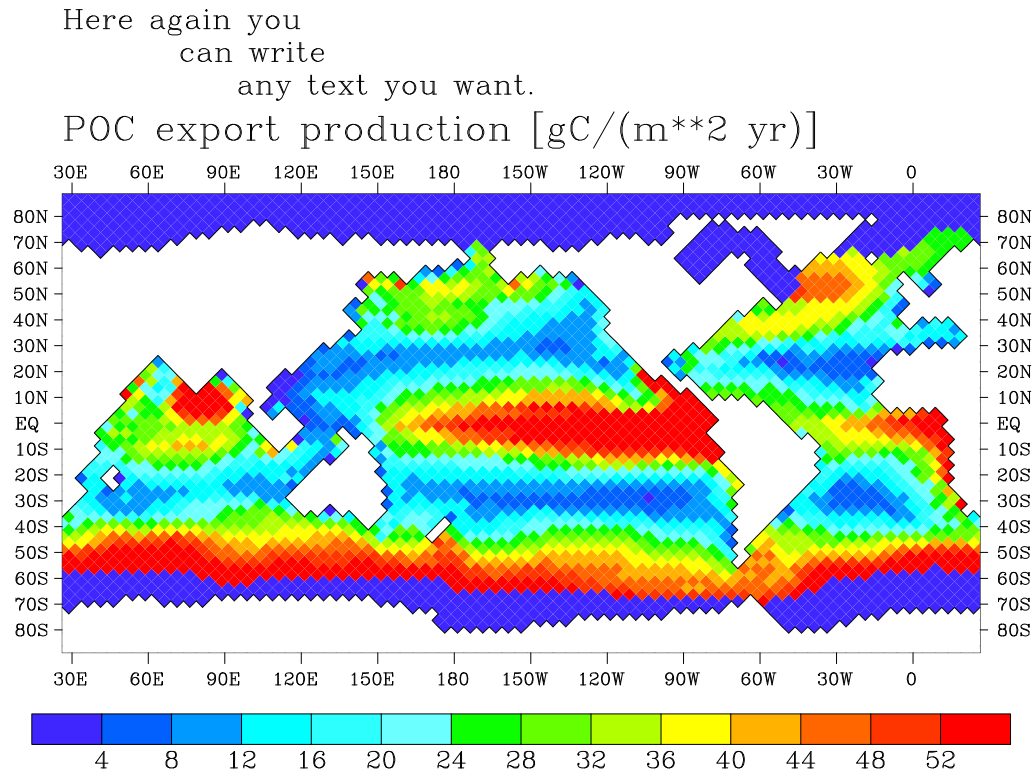


Figure 7: Pixel map (as Fig. 4) with same configuration file as given in Fig. 3 but additional enabling of “1: levelplot pixel”.

[illegible]

Figure 8: Example of file “sets” with selections for a black and white zonal cross section of silicic acid near the equator.

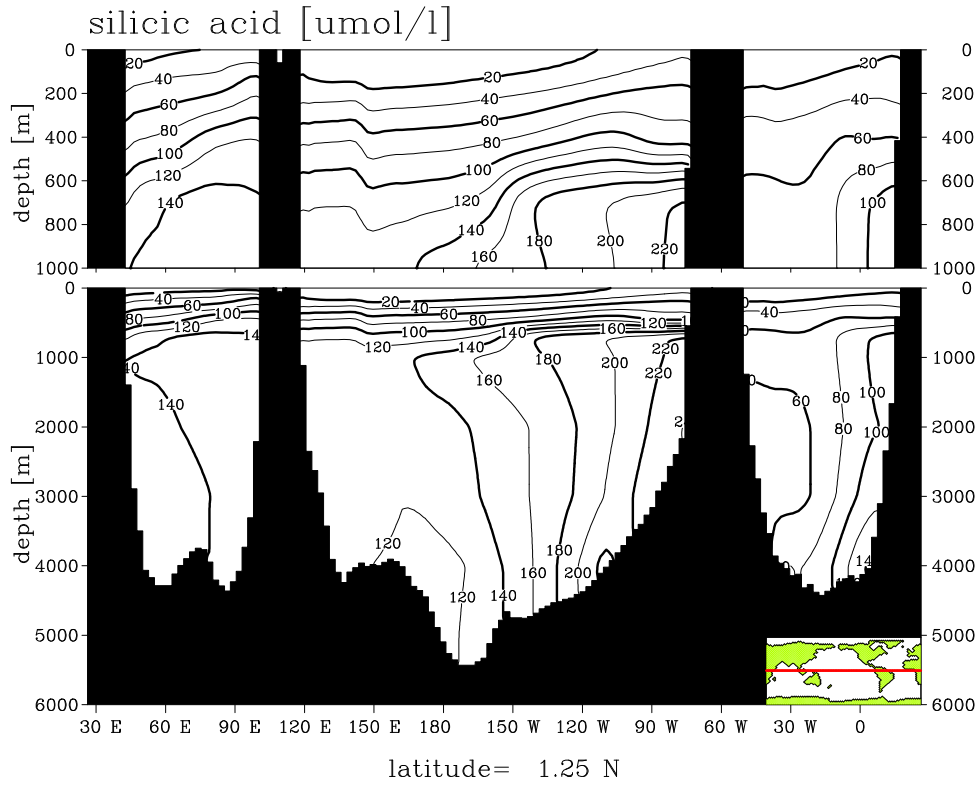


Figure 9: Resulting zonal cross section with specifications from file “sets” as given in Fig. 8.

modelled and observed water column concentrations

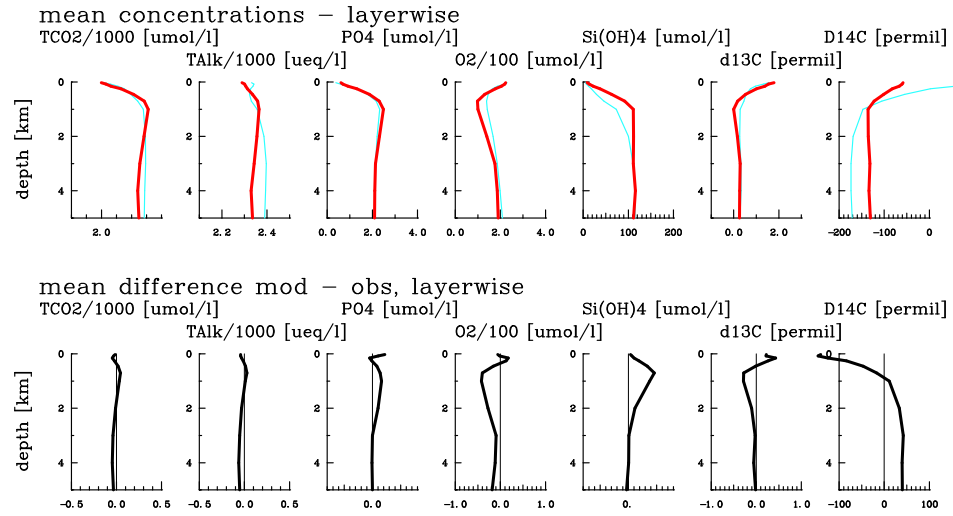


Figure 10: Mean profile plot produced from input file “inventories”. Observed and simulated values were taken both at the same locations. Observed data are from the GEOSECS program.

Figure 11: Example of file “sets” with selections for a single grid point plot.

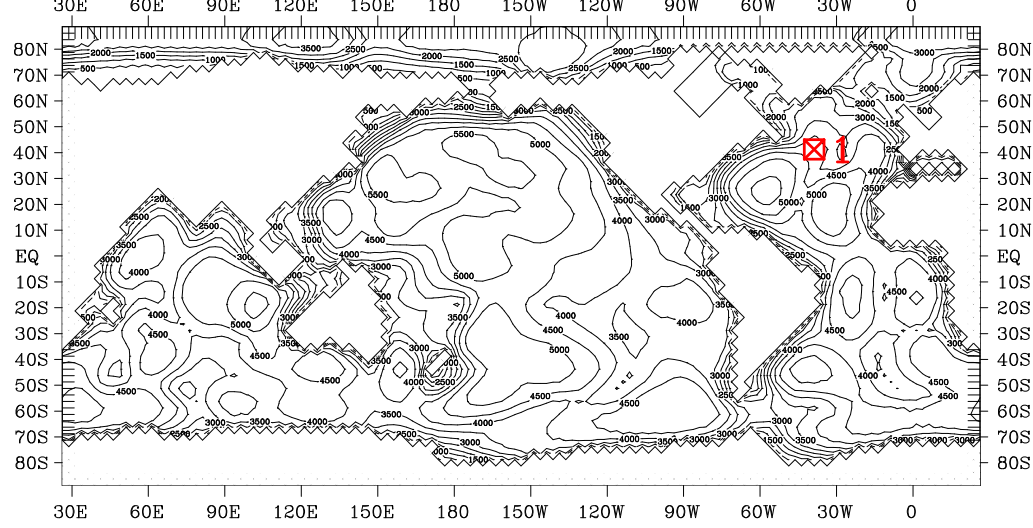
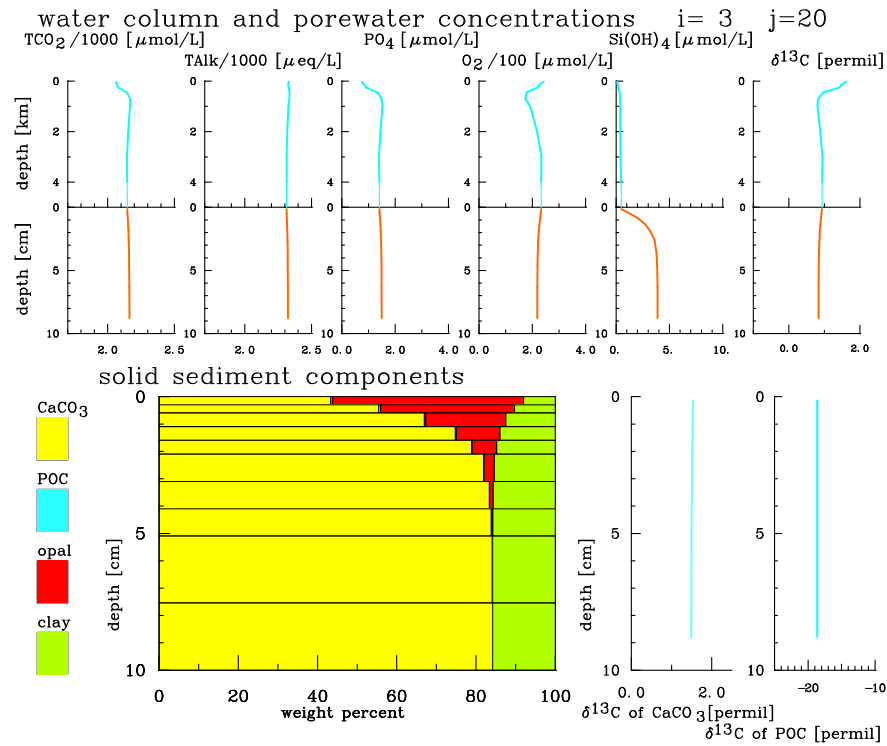


Figure 12: The map shows the position of the grid point at which the single grid point plot of Fig. 13 is produced.



North Atlantic

grid point no. 1

EXAMPLE.

Figure 13: Single grid point plot according to configuration file “sets” from Fig. 11 is produced. See Fig. 12 for the geographical position of this point.

phi	lam	53.105	-177.305	file	3	geopacnis
phi	lam	50.445	-176.583	file	3	geopacnis
phi	lam	44.612	-176.835	file	3	geopacnis
phi	lam	40.770	-176.970	file	3	geopacnis
phi	lam	37.475	-177.322	file	3	geopacnis
phi	lam	32.025	-176.997	file	3	geopacnis
phi	lam	30.567	170.642	file	3	geopacnis
phi	lam	24.992	170.083	file	3	geopacnis
phi	lam	19.017	169.350	file	3	geopacnis
phi	lam	15.400	-176.217	file	3	geopacnis
phi	lam	14.108	-178.633	file	3	geopacnis
phi	lam	12.883	173.467	file	3	geopacnis
phi	lam	12.492	177.435	file	3	geopacnis
phi	lam	5.883	-172.013	file	3	geopacnis
phi	lam	4.562	179.002	file	3	geopacnis
phi	lam	3.385	-177.183	file	3	geopacnis
phi	lam	3.078	178.928	file	3	geopacnis
phi	lam	2.008	178.933	file	3	geopacnis
phi	lam	1.025	178.928	file	3	geopacnis
phi	lam	0.525	178.992	file	3	geopacnis
phi	lam	-0.477	178.983	file	3	geopacnis
phi	lam	-1.033	179.033	file	3	geopacnis
phi	lam	-2.028	179.018	file	3	geopacnis
phi	lam	-2.983	178.983	file	3	geopacnis
phi	lam	-4.567	179.000	file	3	geopacnis
phi	lam	-8.483	-178.095	file	3	geopacnis
phi	lam	-9.192	-169.008	file	3	geopacnis
phi	lam	-10.175	-169.975	file	3	geopacnis
phi	lam	-12.183	-169.900	file	3	geopacnis
phi	lam	-12.680	-175.050	file	3	geopacnis
phi	lam	-13.242	-173.808	file	3	geopacnis
phi	lam	-15.060	-170.377	file	3	geopacnis
phi	lam	-15.217	-170.033	file	3	geopacnis
phi	lam	-15.775	-169.183	file	3	geopacnis
phi	lam	-16.025	-168.478	file	3	geopacnis
phi	lam	-16.697	-167.060	file	3	geopacnis
phi	lam	-17.272	-166.003	file	3	geopacnis
phi	lam	-18.483	-168.050	file	3	geopacnis
phi	lam	-19.255	-171.410	file	3	geopacnis
phi	lam	-20.508	-172.805	file	3	geopacnis
phi	lam	-23.963	-174.520	file	3	geopacnis
phi	lam	-23.977	-175.253	file	3	geopacnis
phi	lam	-24.042	-175.717	file	3	geopacnis
phi	lam	-29.952	-175.730	file	3	geopacnis
phi	lam	-30.025	-176.908	file	3	geopacnis
phi	lam	-30.117	-177.580	file	3	geopacnis
phi	lam	-35.667	-166.783	file	3	geopacnis
phi	lam	-36.520	-179.600	file	3	geopacnis
phi	lam	-37.062	-168.602	file	3	geopacnis
phi	lam	-38.380	-170.070	file	3	geopacnis
phi	lam	-40.508	-166.700	file	3	geopacnis
phi	lam	-41.558	-166.833	file	3	geopacnis
phi	lam	-43.250	-166.767	file	3	geopacnis
phi	lam	-44.183	-171.492	file	3	geopacnis
phi	lam	-44.217	-166.767	file	3	geopacnis
phi	lam	-44.947	-166.658	file	3	geopacnis
phi	lam	-46.000	-166.750	file	3	geopacnis
phi	lam	-46.717	-166.933	file	3	geopacnis
phi	lam	-50.633	-179.983	file	3	geopacnis
phi	lam	-52.583	-178.033	file	3	geopacnis
phi	lam	-54.083	-176.967	file	3	geopacnis
phi	lam	-56.000	-175.583	file	3	geopacnis
phi	lam	-58.017	-174.000	file	3	geopacnis
phi	lam	-61.985	-174.000	file	3	geopacnis
phi	lam	-67.708	-173.983	file	3	geopacnis
phi	lam	-69.300	-173.500	file	4	geopacger

Figure 14: Example of file “cruise_track” - selected stations from which the western Pacific GEOSECS section for dissolved phosphate is compiled.

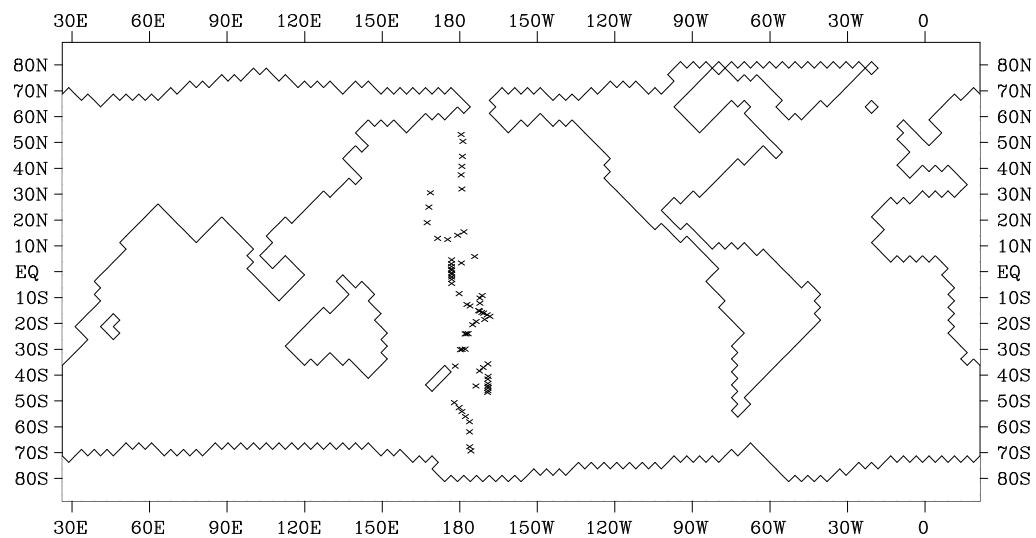


Figure 15: Example for plot produced from file “cruise_track” (see Fig. 14) after having set “1: cruise track check only” in file “sets”.

wpac geos	64	88.750	-176.250	0.000	0.000	---
wpac geos	64	86.250	-176.250	0.000	0.000	---
wpac geos	64	83.750	-176.250	0.000	0.000	---
wpac geos	64	81.250	-176.250	0.000	0.000	---
wpac geos	64	78.750	-176.250	0.000	0.000	---
wpac geos	64	76.250	-176.250	0.000	0.000	---
wpac geos	64	73.750	-176.250	0.000	0.000	---
wpac geos	64	71.250	-176.250	0.000	0.000	---
wpac geos	64	68.750	-176.250	0.000	0.000	---
wpac geos	64	66.250	-176.250	0.000	0.000	---
wpac geos	64	63.750	-176.250	0.000	0.000	---
wpac geos	64	61.250	-176.250	0.000	0.000	---
wpac geos	64	58.750	-176.250	0.000	0.000	---
wpac geos	64	56.250	-176.250	0.000	0.000	---
wpac geos	64	53.750	-176.250	0.000	0.000	---
wpac geos	64	51.250	-176.250	53.105	-177.305	obs
wpac geos	64	48.750	-176.250	50.445	-176.583	obs
wpac geos	64	46.250	-176.250	0.000	0.000	---
wpac geos	64	43.750	-176.250	44.612	-176.835	obs
wpac geos	64	41.250	-176.250	0.000	0.000	---
wpac geos	64	38.750	-176.250	40.770	-176.970	obs
wpac geos	64	36.250	-176.250	37.475	-177.322	obs
wpac geos	64	33.750	-176.250	0.000	0.000	---
wpac geos	64	31.250	-176.250	32.025	-176.997	obs
wpac geos	59	28.750	171.250	30.567	170.642	obs
wpac geos	59	26.250	171.250	0.000	0.000	---
wpac geos	59	23.750	171.250	24.992	170.083	obs
wpac geos	59	21.250	171.250	0.000	0.000	---
wpac geos	58	18.750	168.750	19.017	169.350	obs
wpac geos	61	16.250	176.250	0.000	0.000	---
wpac geos	63	13.750	-178.750	14.108	-178.633	obs
wpac geos	61	11.250	176.250	12.492	177.435	obs
wpac geos	61	8.750	176.250	0.000	0.000	---
wpac geos	62	6.250	178.750	0.000	0.000	---
wpac geos	62	3.750	178.750	4.562	179.002	obs
wpac geos	62	1.250	178.750	2.008	178.933	obs
wpac geos	62	-1.250	178.750	-1.033	179.033	obs
wpac geos	62	-3.750	178.750	-2.983	178.983	obs
wpac geos	62	-6.250	178.750	-4.567	179.000	obs
wpac geos	63	-8.750	-178.750	-8.483	-178.095	obs
wpac geos	67	-11.250	-168.750	-10.175	-169.975	obs
wpac geos	65	-13.750	-173.750	-13.242	-173.808	obs
wpac geos	67	-16.250	-168.750	-16.025	-168.478	obs
wpac geos	67	-18.750	-168.750	-18.483	-168.050	obs
wpac geos	65	-21.250	-173.750	-20.508	-172.805	obs
wpac geos	65	-23.750	-173.750	0.000	0.000	---
wpac geos	64	-26.250	-176.250	-24.042	-175.717	obs
wpac geos	64	-28.750	-176.250	0.000	0.000	---
wpac geos	63	-31.250	-178.750	-30.117	-177.580	obs
wpac geos	66	-33.750	-171.250	0.000	0.000	---
wpac geos	68	-36.250	-166.250	-35.667	-166.783	obs
wpac geos	66	-38.750	-171.250	-38.380	-170.070	obs
wpac geos	68	-41.250	-166.250	-40.508	-166.700	obs
wpac geos	68	-43.750	-166.250	-43.250	-166.767	obs
wpac geos	68	-46.250	-166.250	-46.000	-166.750	obs
wpac geos	68	-48.750	-166.250	-46.717	-166.933	obs
wpac geos	63	-51.250	-178.750	-50.633	-179.983	obs
wpac geos	63	-53.750	-178.750	-52.583	-178.033	obs
wpac geos	64	-56.250	-176.250	-56.000	-175.583	obs
wpac geos	65	-58.750	-173.750	-58.017	-174.000	obs
wpac geos	65	-61.250	-173.750	0.000	0.000	---
wpac geos	65	-63.750	-173.750	-61.985	-174.000	obs
wpac geos	65	-66.250	-173.750	0.000	0.000	---
wpac geos	65	-68.750	-173.750	-67.708	-173.983	obs
wpac geos	65	-71.250	-173.750	-69.300	-173.500	obs
wpac geos	65	-73.750	-173.750	0.000	0.000	---
wpac geos	65	-76.250	-173.750	0.000	0.000	---
wpac geos	65	-78.750	-173.750	0.000	0.000	---
wpac geos	65	-81.250	-173.750	0.000	0.000	---
wpac geos	65	-83.750	-173.750	0.000	0.000	---
wpac geos	65	-86.250	-173.750	0.000	0.000	---
wpac geos	65	-88.750	-173.750	0.000	0.000	---

Figure 16: Example of file “secind_new” - constructed from the positions as given in file “cruise_track” (Fig. 14) by setting “1: fill meridional section” in file “sets”.

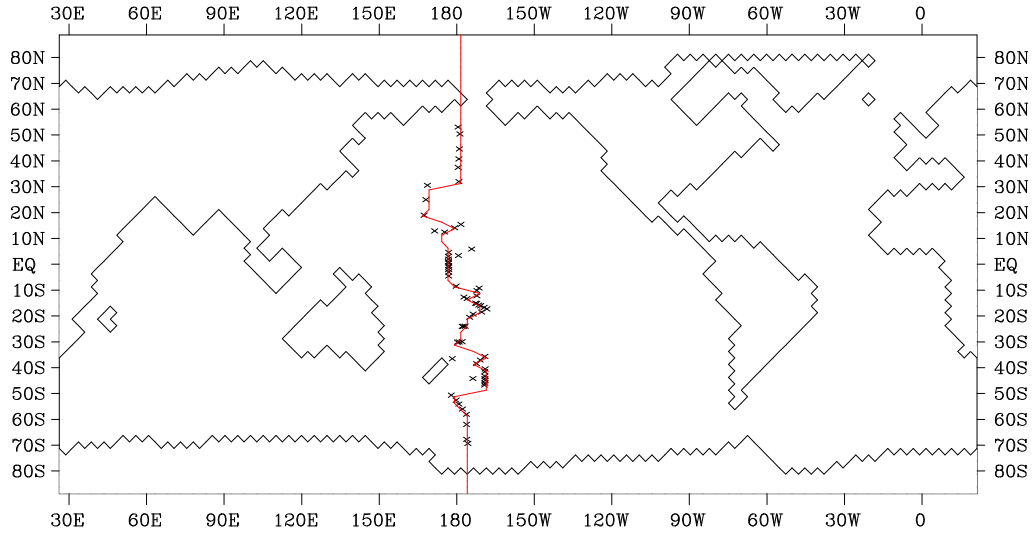


Figure 17: Example for cross section constructed from the station positions in file “cruise_track” (see Fig. 14) through use of option “1: fill meridional section” in file “sets”.

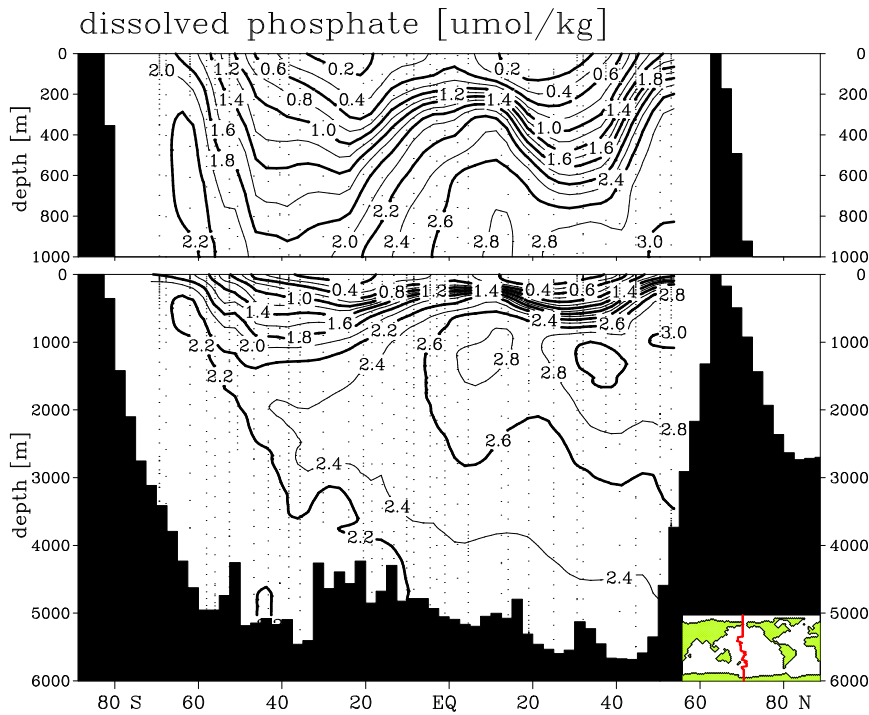


Figure 18: Example for plotting an observed phosphate section.

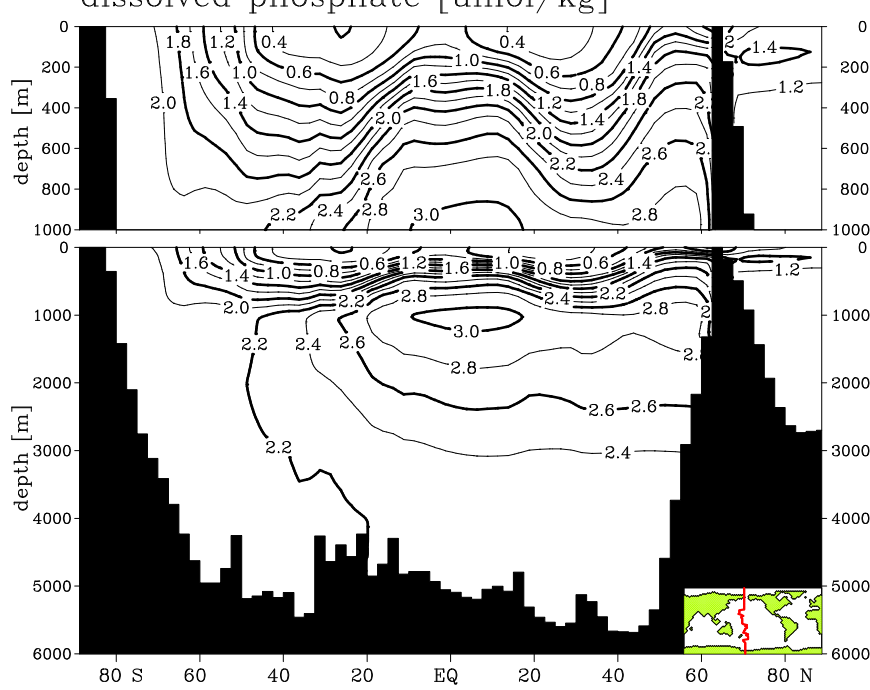


Figure 19: Example for plotting the corresponding model result to Fig. 18.

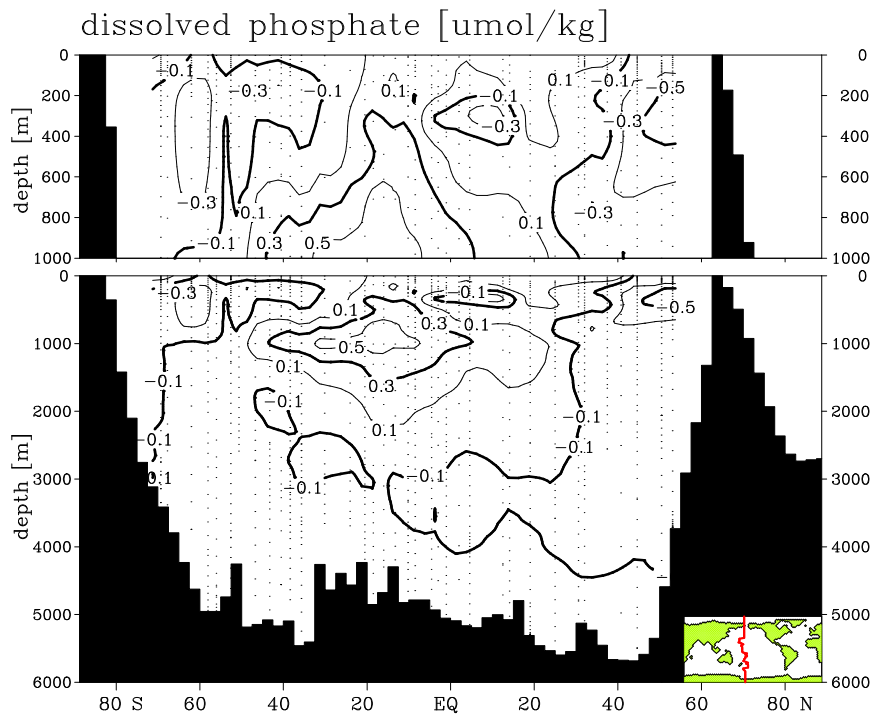


Figure 20: Example for plotting the difference modelled minus observed data corresponding to Figs. 18 and 19.

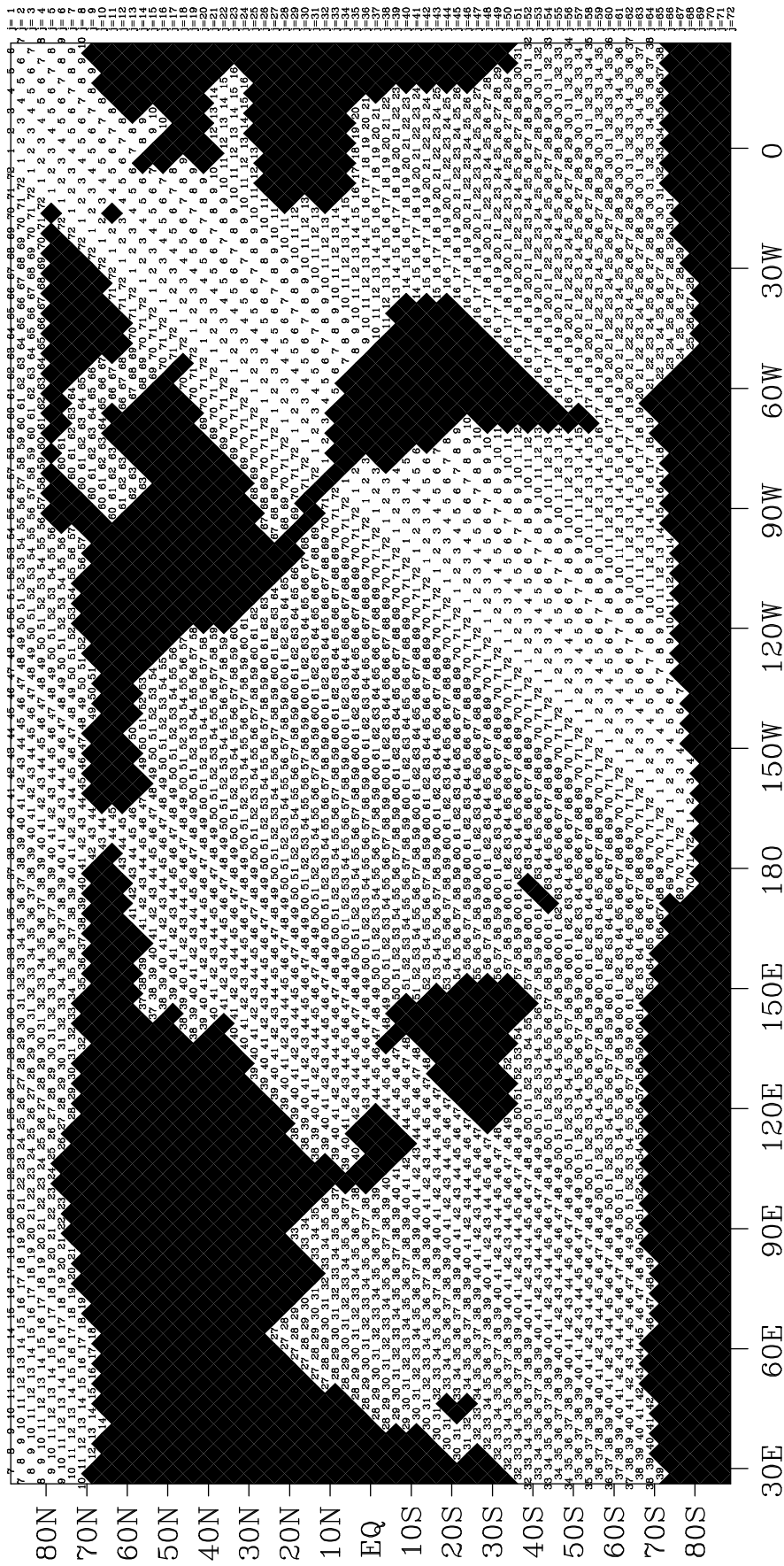


Figure 21: Zonal and meridional indices of the original model grid.