Report No. 5

The Hamburg Ocean Carbon Cycle Circulation Model

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Contents

1.	SU	MMARY PA	AGE	 1
	1.1	MAIN AUT	HORS OF THE MODEL	 1
	1.2	PERSON(S)	RESPONSIBLE FOR MODEL SUPPORT AT THE DKRZ	 1
2.	MO	DDEL DESC	RIPTION (annually averaged version, Cycle 1)	 3
	2.1	DISSOLUTI	ON/INORG. PRECIPITATION OF CACO ₃	. 4
	2.2	ORG. C AN	D CACO ₃ PRIMARY PRODUCTION	 5
	2.3	REMINERA	LIZATION OF ORG. C	 6
	2.4	GAS EXCH	ANGE OCEAN-ATMOSPHERE	 6
			T OF TRACERS WITH OCEAN VELOCITY FIELD	
3			CRIPTION	
٥.				
			ES	
			LES	
	3.3	COMMON-	BLOCKS	 11
	3.4	THE PROG	RAM	 14
		3.4.1 Main	Program	 14
		3.4.2 Subro	outines	 16
		3.4.2.1	Subroutine INITIA1 - initialization of physical fields	 17
		3.4.2.2	Subroutine INITIA2 - initialization of geochemical fields	 17
		3.4.2.3	Subroutine INIBIL - initialization of geochemical inventories	 17
		3.4.2.4	Subroutine BILANZ - check of geochemical matter conservation .	 17
		3.4.2.5	Subroutine POOLS - calculation of carbon pool sizes	
		3.4.2.6	Subroutine LYSOCL - dissolution/inorg. precipitation of CaCO ₃	. 18
		3.4.2.7	Subroutine BIOSOF - org. C and CaCO ₃ primary production	 18
		3.4.2.8	Subroutine OXYCON - remineralization of org. C	 18
		3.4.2.9	Subroutine SURFCH - gas exchange ocean-atmosphere	 18
		3.4.2.10	Subroutine BIOTUR - resuspension of sedimented matter	 18
		3.4.2.11	Subroutine ADVECT - transport of tracers with ocean velocity field	 18
	3.5	PARAMETI	ERS	 19
	36	FLOW CHA	RTS	20

4.	USER'S MANUAL	•	. 2	23
	4.1 HOW TO RUN THE MODEL	•	. 2	23
	4.2 HOW TO GET OUTPUT (PLOTS)	•	. 2	23
5.	REFERENCES	•	. 2	25
\mathbf{A}	opendix A JOB TO PERFORM A MODEL RUN	•	. 2	27
\mathbf{A}	opendix B JOB TO PERFORM PLOTS OF MODEL RESULTS	•	. 2	29
\mathbf{A}	opendix C PLOT OUTPUT EXAMPLES	•	. 3	35
A	opendix D CODE NUMBERS USED BY POSTPROCESSING PACKAGE		. 3	37

1. SUMMARY PAGE

The carbon cycle model calculates the prognostic fields of oceanic geochemical carbon cycle tracers making use of a "frozen" velocity field provided by a run of the LSG oceanic circulation model (see the corresponding manual, LSG = Large Scale Geostrophic).

The carbon cycle model includes a crude approximation of interactions between sediment and bottom layer water. A simple (meridionally diffusive) one layer atmosphere model allows to calculate the CO_2 airborne fraction resulting from the oceanic biogeochemical interactions.

1.1 MAIN AUTHORS OF THE MODEL

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1.2 PERSON(S) RESPONSIBLE FOR MODEL SUPPORT AT THE DKRZ

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2. MODEL DESCRIPTION (annually averaged version, Cycle 1)

The model simulates the inorganic carbon cycle and part of the organic carbon cycle of the World Ocean. Aditionally to the ocean water carbon reservoir the carbon pools of the atmosphere and marine sediment are considered.

The internal redistribution of tracers within the ocean water is based on the velocity field and the thermohaline fields of the dynamical Hamburg Large Scale Geostrophic (LSG) Ocean General Circulation Model. This dynamical model is described by Maier-Reimer et al. (1991). The carbon cycle model uses the same grid as the LSG model (see Maier-Reimer and Mikolajewicz, 1991). The velocity and thermohaline fields are taken from the input files and are not modified by the carbon cycle model.

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 "biological carbon pump" is simulated with its two components - the organic carbon pump and the calcium carbonate counterpump. Phytoplankton organisms grow in the ocean surface layer as a function of the concentration of dissolved biolimiting nutrients in sea water. The soft tissue of the organisms is called particulate organic carbon. Besides organic soft tissue the organisms produce hard parts in the form of calcium carbonate (CaCO₃). The ratio of nutrients to organically bound carbon ("Redfield ratio") and the ratio of calcium carbonate carbon to organically bound carbon ("rain ratio") within the newly formed biogenic material are fixed. The remnants of the planktonic biota sink through the water column. The organic material is remineralized parallel to oxygen consumption. While most of the particulate organic carbon is remineralized within the upper 1000 m of the ocean the CaCO₃ hard parts sink to greater depth before they undergo enhanced degradation by inorganic solution. Superimposed on the production and degradation of biogenic matter is the transport of dissolved and suspended matter by the oceanic velocity field.

Biogenic matter is partly lost to sediment pools for organic carbon and CaCO₃. The cycling of matter in the model is closed by resuspension of sedimented matter back into the water column.

The carbon cycle model includes a simple atmosphere model with only diffusive transport of CO₂ and only in meridonal directions. Gas transfer between ocean and atmosphere is performed via a simple bulk formula.

2.1 DISSOLUTION/INORG. PRECIPITATION OF CACO₃

Degradation of $CaCO_3$ is controlled by the degree of undersaturation of seawater with respect to calcite. The destruction of aragonite (the metastable modification of marine $CaCO_3$) is accounted for in the model by allowing partial destruction of $CaCO_3$ even in cases of calcite supersaturation. After the vertical redistribution of newly produced $CaCO_3$ particles, at first the deviation ΔCO_3 from the saturation concentration is calculated. (Since the calcium concentration in seawater is almost constant and much higher than the CO_3^{2-} concentration, the marine $CaCO_3$ saturation is almost entirely determined by the amount of CO_3^{2-} ions in solution.) Then the amounts of total $CaCO_3$ available in the respective grid box that are dissolved (D_{pot}) or can be precipitated (E) are determined and the concentrations for ΣCO_3 and $CaCO_3$ at the new time level are accordingly:

$$\Delta CO_3 = [CO_3^{2-}]^{t} - [CO_3^{2-}]_{sat}$$
 (2.1.1)

$$D_{pot} = \left[CaCO_3\right]^t \cdot 0.5 \cdot \left(1 - \frac{\Delta CO_3}{c_1 + |\Delta CO_3|}\right)$$
 (2.1.2)

$$E = \max(0, \Delta CO_3) \tag{2.1.3}$$

$$\left[\sum CO_{2}\right]^{t+\Delta t} = \left[\sum CO_{2}\right]^{t} + D_{pot} - c_{2} E$$
 (2.1.4)

$$[CaCO_3]^{t+\Delta t} = [CaCO_3]^t - D_{pot} + c_2 E$$
 (2.1.5)

where

 ΔCO_3 : deviation of carbonate concentration from the saturation value

 $[CO_3^{2-}]$: carbonate concentration at old time level $[CO_3^{2-}]_{sat}$: saturation concentration of carbonate D_{pot} : amount of CaCO₃ that reenters solution E : amount of CaCO₃ that can be precipitated

 $[\sum CO_2]$: total dissolved inorganic CO2 at new and old time levels respectively : calcium carbonate concentration at new and old time levels respectively

c₁, c₂ : adjustable constants (here $c_1 = 10^{-4} \, \mu \text{mol/L}$, $c_2 = 1$ in bottom layer and zero else)

2.2 ORG. C AND CACO₃ PRIMARY PRODUCTION

Here the CaCO₃ production in the surface ocean is calculated. The CaCO₃ production rate is coupled to the particulate organic carbon (POC) new production calculated in the advection step (subroutine ADVECT). After the production of biogenic particulate matter in the surface layer it is redistributed within the water column. Biogenic particulate matter is produced only in the uppermost model layer and is immediately redistributed within the water column in amounts decreasing with depth. The immediate redistribution is a reasonable assumption, because the time scale for the particles sinking through the water column is shorter (about 100 m/day [e.g., Suess, 1980]) than the time step of 1 year. 20% of the CaCO₃ production is assumed to fall immediately to the bottom layer, while the remainder is distributed according to an exponentially decreasing vertical flux:

$$F_{CaCO_3}(z) = (P_{CaCO_3} - S_{CaCO_3}) \cdot e^{(-z/d_p)} + S_{CaCO_3}$$
 (2.2.1)

where

: depth Z

 P_{CaCO_3} : annual production of CaCO₃

: part of P_{CaCO₂} that sinks immediately to the bottom layer (here 20%)

P_{CaCO₃} S_{CaCO₃} d_n : e-folding-depth for CaCO₃ flux (here 4000 m)

By this formulation of the vertical redistribution of newly formed CaCO₃ no degradation of CaCO₃ is included yet, that is performed separately in another step (see below).

POC flux is assumed to follow the 1/z-law after Suess [1980], with a modification of distributing about one third of the POC new production $(28.7\% = P_{POC} - F_1 (50m))$, see below) like the newly formed CaCO₃. This addition is introduced to account for organic material coated by hard shells:

$$F_{POC} = F_1 + F_2 (2.2.2)$$

with

$$F_1 = \frac{P_{POC}}{0.0238 \cdot z + 0.212} \tag{2.2.3}$$

$$F_2 = (P_{POC} - F_1 (50m) - S_{POC}) e^{(-z/d_p)} + S_{POC}$$
 (2.2.4)

where

: depth Z

: annual production of POC P_{POC}

: part of P_{POC} that sinks immediately to the bottom layer (here 5.7%; that is 20% of S_{POC}

those 28.7% of total POC produced that are not considered by the 1/z-formulation

of Suess [1980])

 d_{p} : : e-folding-depth for CaCO₃ flux (here 4000 m)

2.3 REMINERALIZATION OF ORG. C

Remineralization of organic matter and corresponding oxygen consumption are modeled according to a fixed Redfield ratio $P:\Delta O_2$ of 1:-172 [Takahashi et al., 1985]. O_2 concentration is not allowed to become negative. In the case of full O_2 consumption, POC degradation stops at the respective grid point. After the determination of the amount of POC that is remineralized during one time step (ΔPOC) the POC, PO_4 , and O_2 concentrations for the new time level are calculated:

$$\Delta POC = r \cdot min (([O_2]_{min} - [O_2]^t) \cdot R_{Red}, [POC]^t)$$
(2.3.1)

$$[POC]^{t+\Delta t} = [POC]^{t} - \Delta POC$$
 (2.3.2)

$$[PO_4]^{t+\Delta t} = [PO_4]^t + \Delta POC$$
 (2.3.3)

$$\left[O_{2}\right]^{t+\Delta t} = \left[O_{2}\right]^{t} - \frac{\Delta POC}{R_{Red}}$$
 (2.3.4)

where

 ΔPOC : amount of POC that can be remineralized during one time step

r : remineralization rate (here 1.0 year-1 in the surface layer, 0.05 year-1 elsewhere)

 R_{Red} : Redfield ratio P: ΔO_2

 $[O_2]$: oxygen concentration at the new and old time step respectively

 $\left[\mathrm{O}_{2}\right]_{\mathrm{min}}$: threshold value of oxygen concentration for bacterial decomposition

[PO₄] : phosphate concentration at the new and old time step respectively (normalized to

a POC concentration by the Redfield ratio P:C)

[POC] : particulate organic carbon concentration at the new and old time step respectively

2.4 GAS EXCHANGE OCEAN-ATMOSPHERE

Gas exchange between ocean and atmosphere is performed with a simple bulkformula:

$$F = \lambda \cdot (pCO_2(air) - pCO_2(water))$$
 (2.4.1)

where F is the gas exchange flux and λ is the gas exchange coefficient. For λ a value of 19 mol m⁻² yr⁻¹ at 270 ppm is adopted [cf. Broecker et al., 1986].

2.5 TRANSPORT OF TRACERS WITH OCEAN VELOCITY FIELD

All tracers are transported with the ocean velocity field. An upstream formulation of the tracer equation (continuity equation for amount of matter) is applied:

$$\frac{dp}{dt} = -\operatorname{div}(\vec{v} \cdot c) - q \qquad \text{tracer equation}$$
 (2.5.1)

$$\frac{c^{t+\Delta t}-c^t}{\Delta t} = -\sum_{i} v_i \cdot \frac{c_i^{t+\Delta t}-c^{t+\Delta t}}{\Delta x_i} - a \ I_1 \ \frac{V_{max} \ (c^{t+\Delta t})^2}{K_s + c^{t+\Delta t}}$$
 upstream formulation (2.5.2)

where

c : tracer concentration

velocity vector

q : term for sources and sinks

v_i : velocity component in the direction of grid point i

 Δx_i : distance to neighboring grid point i

c_i: tracer concentration at neighboring grid point i

a : 1 if c is nutrient concentration in the surface layer, 0 otherwise

 I_l : light factor (dependent on latitude) V_{max} : maximum velocity of nutrient uptake

 K_s : half saturation constant (PO₄ concentration, where $dc/dt = c \cdot V_{max}/2$)

Uptake of PO_4 as biolimiting nutrient by phytoplankton in the surface layer is the only additional process included in the tracer transport equation (second term on the right-hand side of (2.5.2)). The advection equation is solved iteratively by a single-level scheme. Uptake of nutrients by organisms is included in this equation to allow a shorter time constant for phytoplankton growth compared to the time step of 1 year. All the other chemical interactions are calculated in separate routines (time splitting method).

The biological POC production is assumed to follow Michaelis-Menten kinetics for nutrient uptake (e.g. Parsons and Takahashi, 1973). For the light factor I_l the same latitudinal profile as in Bacastow and Maier-Reimer (1990) is used. It is coherent with the latitudinal distribution of the annual sum of solar radiation incident on the ocean surface layer. For uptake of inorganically dissolved carbon by phytoplankton a Redfield ratio of P/C = 1/122 [Takahashi et al., 1985] is prescribed.

 $CaCO_3$ production is set proportional to the production of POC according to the rain ratio $(C_{CaCO_3}/C_{organic})$ chosen. A maximum of 1/4 is used with strong reduction of calcite production (close to zero) at temperatures below 2 °C.

3. SYSTEM DESCRIPTION

3.1 INPUT FILES

The model is started with initial conditions on four input files in the subroutines INITIA1 and INITIA2:

- 1. velocity field (file "VELOCI")
- 2. geometry (file "DPHILA")
- 3. ocean identifiers (file "MONITO")
- 4. index file for control maps (file "INDLIS")

If the model is re-started an additional input file is needed:

5. re-start file (with actual values of concentrations) (file "RESTART")

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 as given from the dynamical model (LSG).

In the input file with ocean identifiers every grid point has been assigned to a certain code that indicates which grid point lies in which ocean. The code and the corresponding ocean regions are:

1 : northern Atlantic

2 : equatorial Atlantic

3 : southern Atlantic

4 : northern Pacific

5 : equatorial Pacific

6 : southern Pacific

7 : northern Indian Ocean

8 : equatorial Indian Ocean

9 : southern Indian Ocean

N : Arctic Ocean and European Polar Seas

S : Southern Ocean

The re-start file contains the result of the preceding model integration with all basic geochemical fields of all model reservoirs and an indicator for the last year of integration. A file with exactly the same format is produced at the end of the model run (result re-start file, see below).

3.2 OUTPUT FILES

Four output files are produced by the model and are saved after a run:

- job flow control file (dependent on run mode, standard output, written on file "TAPE6" or "OUTPUT")
- result re-start file ("RESULT")
- postprocessor input file ("POSTIN")
- profile file ("PROFIL")

The job flow control file contains all control prints and all information about the job flow and the performance of the integration. All error messages are given here. During the integration continuous information about the conservation of the chemical inventories, the number of iterations (in the advection algorithm), the year of integration, and the atmospheric CO₂ partial pressure is provided. At the end of the run the actual values for new production of particulate organic carbon and calcium carbonate and the carbon pool inventories (atmosphere, ocean, sediment) are printed. Finally, line printer plots of three different meridional (western Atlantic, western Pacific, eastern Pacific) are produced that help to interprete the result. Examples for plot output are given in Appendix C.

The result re-start file contains the result of the model integration with all basic geochemical fields of all model reservoirs and an indicator for the last year of integration. From this basic file all relevant variables of the simulation can be derived. This essential file is saved at the end of an integration.

The postprocessor input file contains the fields that can be analysed after a model run. Besides the geochemical fields stored in ta similar way to the re-start file it includes derived quantities as e.g. the primary production rate, the CO_3^{2-} ion concentration, the difference in CO_2 partial pressure between atmosphere and ocean etc.... One header line with basic information is preceding every array. From the postprocessor input file plots can be produced using of the postprocessor PLOFIL and the plot programs SECPLC and MAPPLC.

The profile file contains mean depth profiles of different geochemical quantities and specific ocean regions. This file is the input file for program LYPROF which plots those depth profiles together with corresponding observed depth profiles from the GEOSECS expedition.

3.3 COMMON-BLOCKS

The COMMON-blocks are summarized in four different COMDECKS:

COMDECK BLOCK

COMDECK V12MNMT

COMDECK V12MNM2

COMDECK CACO3C

Every variable of the COMMON-blocks is documented in the program header. Therefore a full list of the variables is not repeated here.

In general following notation is used throughout the model:

- I: zonal direction
- J: meridional direction
- K: vertical direction

In COMDECK BLOCK the array boundaries for the model grid (horizontal and vertical resolution) and the number of tracers (geochemical variables) are stored:

- IE: number of grid points in zonal direction (longitude bands)
- JE: total number of grid points in meridional direction (latitude bands)
- KE: number of grid points in vertical direction (layers)

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

- JL1: first latitude band index (northern boundary of model domain) that contains valid information for the chemical variables
- JLE: last latitude band index (southern boundary of model domain) that contains valid information for the chemical variables

Finally, with parameter NV the number of geochemical key variables is specified.

Example:

If the model has a 72x72 grid points horizontal resolution, 11 layers, and 12 geochemical key variables we have to specify

The geochemical key variables for ocean and atmosphere are contained in COMDECK V12MNMT. For mnemotechnical reasons all variables have two different names (introduced by EQUIVALENCE statements): one that shows the actual meaning of the variable, and one that allows to handle the variables easily in DO loops.

For atmospheric CO₂ the three carbon isotopes ¹²CO₂, ¹³CO₂ and ¹⁴CO₂ are specified by the mnemotechnical names and DO loop names:

Quantity	<u>Variable</u>	DO loop variable
$^{12}CO_2$	ATC12(I,J)	ATC(I,J,1)
$^{13}CO_{2}^{-}$	ATC13(I,J)	ATC(I,J,2)
$^{14}\text{CO}_2$	ATC14(I,J)	ATC(I,J,3)

The geochemical variables for seawater are represented by the following mnemotechnical names and the DO loop names:

Quantity	<u>Variable</u>	DO loop variable
$\Sigma^{12}CO_2$	SCO212(I,J,K)	CA(I,J,K,1)
total alkalinity	ALKALI(I,J,K)	CA(I,J,K,2)
dissolved phosphate	PHOSPH(I,J,K)	CA(I,J,K,3)
dissolved oxygen	OXYGEN(I,J,K)	CA(I,J,K,4)
POC (12C)	POC12(I,J,K)	CA(I,J,K,5)
$CaCO_3$ (^{12}C)	CALC12(I,J,K)	CA(I,J,K,6)
$\Sigma^{13}CO_2$	SCO213(I,J,K)	CA(I,J,K,7)
$\Sigma^{14}CO_2$	SCO214(I,J,K)	CA(I,J,K,8)
POC (13C)	POC13(I,J,K)	CA(I,J,K,9)
POC (14C)	POC14(I,J,K)	CA(I,J,K,10)
$CaCO_3$ (^{13}C)	CALC13(I,J,K)	CA(I,J,K,11)
CaCO ₃ (14C)	CALC14(I,J,K)	CA(I,J,K,12)

After having written these variables to the result re-start file after a model run further derived quantities are calculated from these variables and stored in the same arrays that now get new mnemotechnical names via an additional EQUIVALENCE statement according to COMDECK V12MNM2:

<u>Old name</u>	New name
CA(I,J,K,1)	SUPSAT(I,J,K)
CA(I,J,K,2)	PHVALU(I,J,K)
CA(I,J,K,3)	CARION(I,J,K)
CA(I,J,K,4)	SOLPRO(I,J,K)
CA(I,J,K,5)	PREPHO(I,J,K)
CA(I,J,K,6)	not used
CA(I,J,K,7)	not used
CA(I,J,K,8)	not used
CA(I,J,K,9)	not used
CA(I,J,K,10)	not used
CA(I,J,K,11)	not used
CA(I,J,K,12)	not used

Several calcium carbonate cycle relevant quantities and the $CaCO_3$ and organic carbon sediment pool values are found in the last COMDECK CACO3C:

Quantity	<u>Variable</u>
CO ₃ ²⁻ ion concentration	CO2(I,J,K)
H ⁺ ion concentration	HI(I,J,K)
CaCO ₃ (12C) sediment pool	CCSD12(I,J,K)
CaCO ₃ (¹³ C) sediment pool	CCSD13(I,J,K)
CaCO ₃ (¹⁴ C) sediment pool	CCSD14(I,J,K)
POC (12C) sediment pool	OCSD12(I,J,K)
POC (13C) sediment pool	OCSD13(I,J,K)
POC (14C) sediment pool	OCSD14(I,J,K)

3.4 THE PROGRAM

Throughout this program 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.

3.4.1 Main Program

The main program "RUN001" is divided into three parts:

- initialization
- time stepping loop
- output

Most of the computing time is consumed 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 stepping loop. Only the advection algorithm (transport of substances with the ocean velocity field) and the extraction of biolimiting nutrients from the surface layer are carried out parallel in one subroutine.

The main program begins with a header containing basic general information about the program which in part is also given in this manual. The header includes a schematic overview over the model grid, a flow chart of the program, numbers of the input/output units, references of literature sources relevant for the model, an index of all variables that are used in the main program and in the COMMON-blocks of the COMDECKS with indication of the variable type.

At the beginning of the FORTRAN code the LOGICAL variable RSTART is defined. If RSTART is of value .TRUE., the model run is a re-start run and a re-start file is needed as additional input file. If RSTART is of value .FALSE. no values are read from a re-start file (even if it had been opened) and the initial values of the integration are used as given in the subroutines INITIA1 and INITIA2.

The arrays UFF, TD, XX, XB, DLA, DLRO, and DLRU are needed for the meridional diffusive transport of CO₂ in the atmosphere.

Following files are opened for input and output:

- unit No. 38 file "VELOCI" (input)
- unit No. 36 file "DPHILA" (input)
- unit No. 17 file "MONITO" (input)
- unit No. 83 file "RESTART" (input)
- unit No. 43 file "INDLIS" (input)
- unit No. 87 file "RESULT" (output)

- unit No. 88 file "POSTIN" (output)
- unit No. 19 file "PROFIL" (output)

Several counters concerning the time of integration are set:

The counter for Julian years is initialized by setting the variable ANNU. This variable counts every year of integration. Via ANNU certain input functions (anthropogenic CO₂ input, e.g.) can be activated at given years.

Time step counter NYETOT counts the total number of time steps of an integration. It is set to zero at the start. NYETOT is overwritten during re-start runs when read from the re-start file.

Variable INTSTP specifyies the number of time steps to be integrated. For INTSTP=1 the time loop (see below) is carried out only once.

The variable TIMAX sets the maximum cpu time in seconds that is allowed to be used during the model run. By setting TIMAX to an appropriate value the integration is stopped properly in the case that the run approaches the cpu time limit. The run may not reach the number of integration time steps that are specified by variable INTSTP but saves that part of the required integration that has been produced up to the cpu threshold value TIMAX. The rest of the integration can be carried out afterwards by an additional re-start of the program.

With the statement DO 1111 ... the program enters the time loop and starts simulation of the various biogeochemical processes by subsequent call of subroutines for the different processes. Before the end of the time stepping loop the meridional transport of the different isotopes of CO_2 in the atmosphere is performed.

After having finished the time loop (at statement 1111 CONTINUE) a final calculation of the various carbon pool sizes (CALL POOLS) and the inventories (CALL BILANZ) is carried out and all geochemical key variables are written to the result re-start file.

The main program ends with CLOSE statements for the files attached during the run.

3.4.2 Subroutines

Two subroutines are called for initiation of variables and tunable parameters. In subroutine INITIA1 the velocity field and the geometrical variables, in subroutine INITIA2 the biogeochemical variables are initialized.

The vertical velocity component is calculated newly from the horizontal velocities using the continuity equation.

Now LOGICAL varibale RSTART is set. If RSTART is set .TRUE. the time step counter NYETOT and all relevant geochemical key values are read from the re-start file. If RSTART is set .FALSE. a complete new-start of the model is performed. Modifications in geochemical inventories can be made easily just after the READ statement for the re-start file (i.e. before the radiocarbon production rate is calculated).

After having fixed all geochemical inventories after reading of the re-start values the production rate for radiocarbon is calculated. It is set equal to the amount of radiocarbon that decays in the total model system during one time step.

The inventory check is initated by call of subroutine INIBIL where all chemical inventories are fixed at the beginning of the model run without having modified one of the variables in any way by the simulation of the various processes. The resulting inventories serve as a reference for subsequent checks of conservation of matter during the model run.

Variable IFULBI should be set to zero usually. In this case subroutine BILANZ, that checks conservation of matter, will be called only once per time step. If IFULBI=1 is set, the model inventories are checked after each subroutine.

Subroutine POOLS is called once before the time stepping loop. It prints actual values of the carbon pool sizes for the different reservoirs. Aditionally it can be called at arbitrary positions of the main program. Most useful is to call POOLS at the beginning or end of one or several time steps, at least once at the beginning and at the end of an integration.

The postprocessor input file is prepared in subroutine TRN860. In this part of the program also derived quantities are calculated based on the geochemical key variables and a suite of control output is produced to provide a quicklook onto the model results (line printer plots). Subroutine POIPRO is called in order to give depth profiles of geochemical tracers for special regions of the model ocean.

3.4.2.1 Subroutine INITIA1 - initialization of physical fields

The geometrical parameters (areas, volumes) are set.

The velocity field of the dynamical ocean model is read from the input file via subroutine REACIR. In subroutine REACIR the velocity, layer thickness, convective adjustment, temperature, salinity, topography and ice thickness arrays are read from file VELOCI prepared by the standard I/O as described in Maier-Reimer and Mikolajewicz (1991).

The values of $\Delta \phi$ and $\Delta \lambda$ of the geographical boundaries of the grid point boxes are read from file "DPHILA".

Furthermore the following parameters are specified in this routine: the time step (DT), the decay rate for ¹⁴C during one time step (DECCON), and the diffusion coefficient (DIFF) for the advection routine (see Subroutine ADVECT).

3.4.2.2 Subroutine INITIA2 - initialization of geochemical fields

Currently this routine performs the initialization of the meridional transport of CO₂ in the atmosphere.

The biological parameters and chemical inventories are set in subroutine BIOINI.

The inorganic chemistry varibles and constants are initialized in subroutine CHEMIN.

3.4.2.3 Subroutine INIBIL - initialization of geochemical inventories

The model inventories for each geochemical variable and each reservoir as well the total model inventories for each substance (except oxygen) are calculated. These total inventories are used as reference for the subsequent check of conservation of matter by subroutine BILANZ. The variables C12INV, C13INV, C14INV, PHOINV, and ALKINV represent the total inventories of ¹²C, ¹³C, ¹⁴C, total alkalinity, and phosphate in the model. These values have to be conserved during the integration. The oxygen inventory is allowed to fluctuate according to the amount of oxygen needed for remineralization of organic matter and according to the solubility at the see surface. The ocean oxygen inventories are assumed to be compensated by corresponding changes in the atmospheric oxygen content which is not modelled here.

3.4.2.4 Subroutine BILANZ - check of geochemical matter conservation

BILANZ can be called at any position of the program (of course NOT inside of I,J,K DO loops) to check conservation of matter (12 C, 13 C, 14 C, total alkalinity). If IFULBI:=1 in the main program BILANZ is called after every subroutine call in the time loop (DO 1111) in the main program. If IFULBI:=0 in the main program BILANZ is only called once in each time step (only after the ADVECT routine).

3.4.2.5 Subroutine POOLS - calculation of carbon pool sizes

POOLS calculates the actual values of new production of organic matter (POC) and calcite (CaCO₃) and the carbon contents of the various reservoirs. This routine can be called at any instance within the main program.

$\underline{\textbf{3.4.2.6}} \quad \underline{\textbf{Subroutine LYSOCL - dissolution/inorg. precipitation of CaCO}_3}$

Calculation dissolution and inorganic precipitation of CaCO₃ according to section 2.1.

3.4.2.7 Subroutine BIOSOF - org. C and CaCO₃ primary production

Here the CaCO₃ production in the surface ocean is calculated. The CaCO₃ production rate is coupled to the POC new production calculated in the advection step (see Subr. ADVECT). After the production of biogenic particulate matter in the surface layer it is redistributed within the water column. Biogenic particulate matter is produced only in the uppermost model layer and is immediately redistributed within the water column in amounts decreasing with depth.

By this formulation of the vertical redistribution of newly formed CaCO₃ no degradation of CaCO₃ is included yet, that is performed separately (see section 2.2).

3.4.2.8 Subroutine OXYCON - remineralization of org. C

Remineralization of organic matter and corresponding oxygen consumption are modeled according to a fixed Redfield ratio . O_2 concentration is not allowed to become negative. In the case of full O_2 consumption, POC degradation stops at the respective grid point. After the determination of the amount of POC that is remineralized during one time step (Δ POC) the POC, PO₄, and O₂ concentrations for the new time level are calculated.

3.4.2.9 Subroutine SURFCH - gas exchange ocean-atmosphere

Gas exchange between ocean and atmosphere is performed with the bulkformula (2.4.1).

3.4.2.10 Subroutine BIOTUR - resuspension of sedimented matter

The system of cycling constituents is closed here by resuspension of sedimented matter into the bottom layer at a fixed rate proportional to the sediment content of the respective grid cell. Resuspension occurs in reality due to bioturbation in the uppermost sediment.

3.4.2.11 Subroutine ADVECT - transport of tracers with ocean velocity field

Calculation of the advection of tracers with the 3-D ocean circulation field using an upstream formulation of the tracer equation (see section 2.5).

3.5 PARAMETERS

In namelist TUNE the following constants and variables can be set individually by the user:

- INTSTP(=3) : number of time steps ($\Delta t = 1$ year)
- TIMAX(=1200.): maximum CPU-time in seconds

Changes in the geophysical parameters must be done very carefully in the model source code. Please contact the authors for such changes, because a new spin-up of the carbon cycle model might be necessary.

3.6 FLOW CHARTS

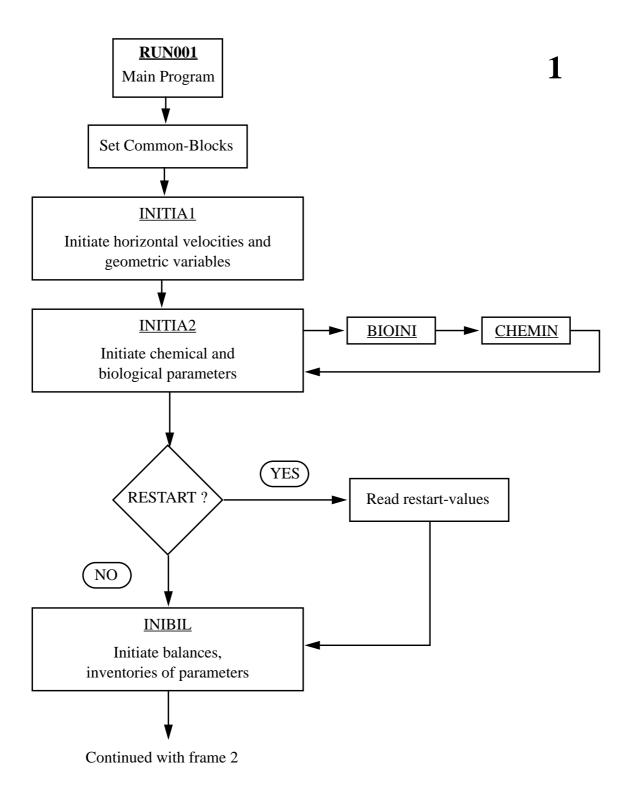


Figure 1 Flow chart of the Hamburg Oceanic Carbon Cycle Model (Part 1)

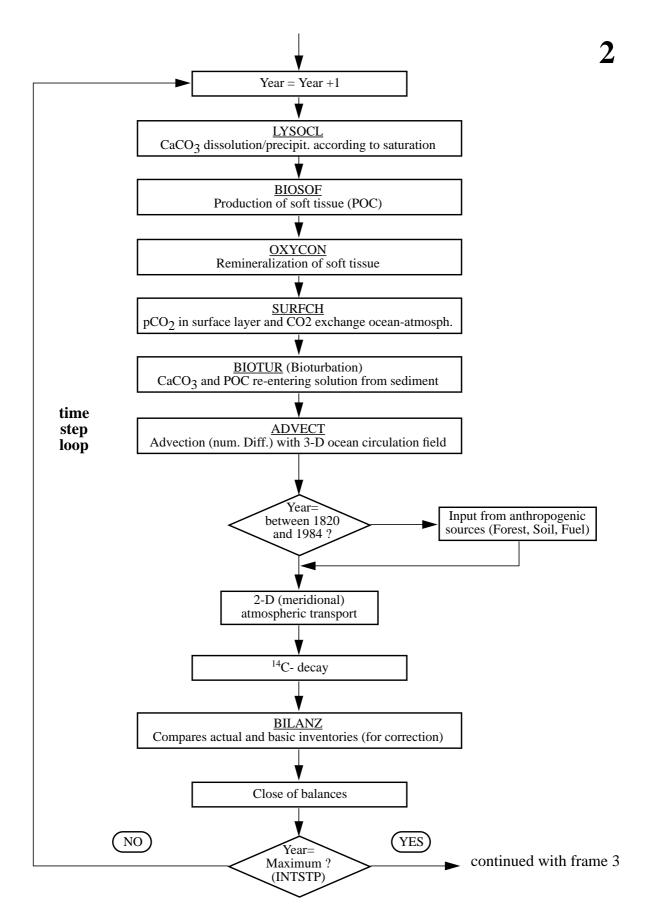


Figure 2 Flow chart of the Hamburg Oceanic Carbon Cycle Model (Part 2)

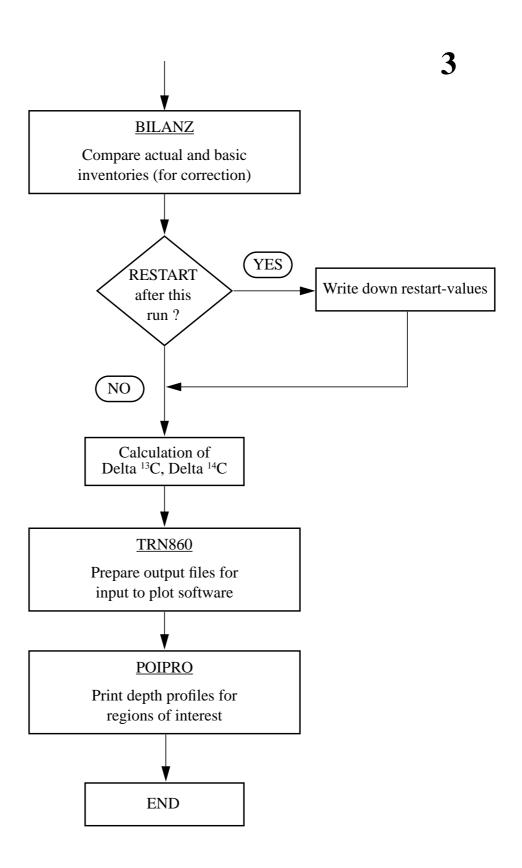


Figure 3 Flow chart of the Hamburg Oceanic Carbon Cycle Model (Part 3)

4. USER'S MANUAL

4.1 HOW TO RUN THE MODEL

An example Bourne-Shell script is available on the Hamburg-CRAY2S. The full path for this script is

/pool/POST/carun.job

To perform this script, copy it wherever you like on your /pf-directory. After doing this you have to change the **outdir** parameter, which should be the path to your personal output directory on the /mf-disk. For user m222222 a possible choice would be:

outdir=/mf/m/m222222/carbon_out

Beware that this directory exists. For further explanations look at the copy of the script, which is shown in Appendix A.

4.2 HOW TO GET OUTPUT (PLOTS)

In principle, there is a vast number of possible applications of the model. So the output processing presented here is only a small part of many possible options that might be required. However, the way the output is handeled here, should enable you to easily add your individual programs in analysing the results. Three program(/-packages) are offered here:

- Iyprof produces mean depth profiles of δ¹⁴C (rel. to the model atmosphere value), PO₄, dissolved O₂, ΣCO₂, and alkalinity of the model provinces Tropical Pacific, Antarctica, Northern Atlantic, Southern Atlantic, Northern Indian Ocean, Tropical Indian Ocean, Southern Indian Ocean, Tropical Atlantic, Southern Pacific, and Northern Pacific and plots the respective mean profile of the GEOSECS data for a quick look of the model results.
- 2. **plofil11** is the interface between the main model postprocessor input file POSTIN and further treatment of the model results. POSTIN contains all relevant parameters of the model run together in one file using the same standard format as the LSG-model output (for code numbers of the geochemical parameters see Appendix D). This file is written in binary form (Standard Fortran unformatted I/O). The carbon isotope values are uncalibrated in this file. Program **plofil11** cuts file POSTIN into single formatted files (E10.4) for each parameter and calibrates the rare carbon isotopes for atmospheric values of $\Delta^{14}C = 0.0/00$ and $\delta^{13}C = -6.5.0/00$. The resulting small parameter files are preceded by one header line. These files serve as input files for the plotting routines. You may make use of these files for your individual treatment of the model results as well. The plot routines now have to read only that parameter array that has to be plotted.
- 3. Plot routines for merdional cross sections **sec11** and **sec11_bw** and for horizontal maps **map11** and **map11_bw** (for colour and b+w plots). You have the choice of four different cross sections close to the GEOSECS sections eastern/western Atlantic/Pacific. Every level of the model can be plotted inidividually with the map routines.

All three postprocessing utilities reside as FORTRAN programs at the CRAY2S in the directory

/pool/POST/carbon

An example Bourne-Shell script is provided by

/pool/POST/capost.job

To perform this script, copy it wherever you like on your /pf-directory. After doing this you have to change the **outdir** parameter, which should be the path to your personal output directory on the /mf-disk, as decribed in section 4.1.

For further explanations look at the copy of the script, which is shown in Appendix B.

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Appendix A JOB TO PERFORM A MODEL RUN

```
# QSUB-q M4
# QSUB-eo
                              # standard error und output
# QSUB-r car
                              # process-name
# QSUB
set -x
outdir=/mf/b/k204002/outcarb
moddir=/pool/POST/carbon
cd STMPDIR
#set -e
                             # execution of script will be aborted if error occurs
ja jacct
#
    New start from quasi steady state produced with standard
    velocity field
cp $moddir/RESTART1 RESTART
    Restart from previous run
#cp $outdir/RESULT RESTART
#
    Model forcing
    standard output from lsg_ogcm1 (annual mean)
cp $moddir/ST5499M VELOCI
    ocean basin identifiers
cp $moddir/MONITO MONITO
    geometrical variables (from lsg_ogcm1)
cp $moddir/DPHILA DPHILA
    indices and wet points
cp $moddir/INDLIS INDLIS
ls -l
#---
    namelist for model input
cat > INPUT1 << EOF1
&TUNE INTSTP=3,TIMAX=1200.,&END
EOF1
#
#
    INTSTP - number of time steps in this run (DT= 1 year)
    TIMAX - max. of CPU-time in sec. for this run
#
cp $moddir/cc_ogcm1.run .
cc_ogcm1.run < INPUT1 # start carbon cycle model
#
    copy model output and restart file
    PROFIL - mean GEOSECS profils
#
    POSTIN - input for postprocessing
    RESULT - restart file
cp PROFIL POSTIN RESULT $outdir
ls -l
ja -cfs jacct
cd $outdir
pwd
Îs -l
exit
```

Appendix B JOB TO PERFORM PLOTS OF MODEL RESULTS

```
# QSUB-q S3
                            # zeit limit
# QSUB-eo
                            # standard error und output
# QSUB-r cap
                            # process-name
# QSUB
set -x
outdir=/mf/b/k204002/outcarb
moddir=/pool/POST/carbon
cd STMPDIR
    split output of cc_ogcm1 into separate files ("plofil11")
#
cp $moddir/POSTIN POSTIN # output corresp. to stand. restart
cp $moddir/plofil11.f plofil11.f
cf77 -Wf"-e mcx" plofil11.f -o plofil11.run
plofil11.run
                            # execute program
#cp ALKA $outdir/ALKA
#cp ATMOS $outdir/ATMOS
#cp BOTOPP $outdir/BOTOPP
#cp BOTOPU $outdir/BOTOPU
#cp CALC13 $outdir/CALC13
#cp CALC14 $outdir/CALC14
#cp CALCIT $outdir/CALCIT
#cp CALPRO $outdir/CALPRO
#cp CALSED $outdir/CALSED
#cp CO2SUR $outdir/CO2SUR
#cp CO3 $outdir/CO3
#cp DC13 $outdir/DC13
#cp DC14 $outdir/DC14
#cp DDZINT $outdir/DDZINT
#cp DISC3 $outdir/DISC3
#cp DISS3 Soutdir/DISS3
#cp DMIN3 $outdir/DMIN3
#cp KSP $outdir/KSP
#cp O2 $outdir/O2
#cp OADIFF $outdir/OADIFF
#cp ORGSED $outdir/ORGSED
#cp PH $outdir/PH
#cp PHSURF $outdir/PHSURF
#cp PO4 $outdir/PO4
#cp PO40 $outdir/PO40
#cp POC $outdir/POC
#cp POCC13 $outdir/POCC13
#cp POCC14 $outdir/POCC14
#cp S $outdir/S
#cp SATCO3 $outdir/SATCO3
#cp SCO2 $outdir/SCO2
#cp SEALAN $outdir/SEALAN
#cp SOFPRO $outdir/SOFPRO
#cp T $outdir/T
#cp U $outdir/U
#cp V $outdir/V
#cp W $outdir/W
#cp PM $outdir/PM
#cp C14AGE $outdir/C14AGE
```

```
#cp SIO4 $outdir/SIO4
                           PLOTTINGPART
DEVICE=SUNC # versat,PK1,ecolor,tcolor,SUN,SUNC,psm2,pscm1,psz1
case $DEVICE in
    SUN | sun | SUNC | sunc)
                           cp /pf/m/m211021/plot/calc_cg calc
                           cp /pf/m/m211021/plot/mpaint_SUN.o mpaint ;;
                           cp/pf/m/m211021/plot/calc_cg calc ;;
esac
#
#
    get plot-library for ocan data
cp/pf/m/m211021/plot/oplib6 oplib
#
    get definition-library.
case $DEVICE in
    tcolor | ecolor | SUNC | sunc | pscm1) cp /pf/m/m211021/plot/deflibcn deflib ;;
                                     cp/pf/m/m211021/plot/deflib deflib;;
esac
#
    compile, link and run the plot program
#
    Plot GEOSECS profiles ("lyprof") --> quicklook
#
cp $moddir/PROFIL PROFIL
cp $moddir/lyprof.f PLOPRG
cp $moddir/lyprof.dat INP
cft77 PLOPRĞ
case $DEVICE in
    SU* | su*) segldr -o runplo1 PLOPRG.o -lgksg -lncarg -lncarg_no calc mpaint oplib deflib ;;
              segldr -o runplo1 PLOPRG.o -lgksg -lncarg -lncarg_no calc oplib deflib ;;
esac
runplo1 < INP
# result: gksm77.txt
cat PROTOK
cat GKS ERROR
#
    Plot GEOSECS cross sections ("sec11/sec11_bw")
cat > SECINP << EOF1
INPUT FILE FOR PLOTTING VERTICAL CROSS SECTIONS FROM OUTPUT OF CMODEL
TITLE='TEST'
TYPE OF CROSS SECTION
                                                          : YES=1, NO=0
ATLANTIC1
                                                                 (WESTERN ATLANTIC)
                                                          : 1
ATLANTIC2
                                                          : 0
                                                                 (EASTERN ATLANTIC)
PACIFIC1
                                                                 (WESTERN PACIFIC)
                                                          : 1
PACIFIC2
                                                                 (EASTERN PACIFIC)
                                                          : 0
                                                          : YES=1, NO=0
PARAMETER
```

```
CNAME(1)='TOTAL CO2 [(MOLES/LITER)*10**-6] '
                                                            : 1
CNAME(2)='ALKALINITY [(EQUIVALENTS/LITER)*10**-6] 'CNAME(3)='PHOSPHATE [(MOLES/LITER)*10**-6] '
                                                            : 1
CNAME(4)='DISSOLVED OXYGEN [(MOLÉS/LITER)*10**-6] '
CNAME(5)=POC[(MOLES/LITER)*10**-6]
                                                            : 0
CNAME(6)='CALCITE [(MOLES/LITER)*10**-6] '
                                                            : 0
CNAME(7)='DELTA 13C
                                                            : 1
CNAME(8)='DELTA 14C
                                                            : 1
CNAME(9)='POC DELTA 13C'
                                                            : 0
CNAME(10)='POC DELTA 14C'
                                                            : 0
CNAME(11)='CALCITE DELTA 13C'
                                                            : 0
CNAME(12)='CALCITE DELTA 14C'
                                                            : 0
CNAME(13)='DEGREE OF [CO3--] SATURATION [PERCENT] '
                                                            : 0
CNAME(14)='PH-VALUE
                                                            : 0
CNAME(15)='[CO3--][(MOLES/LITER)*10**-6]'
                                                            : 0
CNAME(16)='SOLUBILITY PRODUCT
                                                            : 0
CNAME(17)='PREFORMED PO4 [(MOLES/LITER)*10**6] '
                                                            : 0
CNAME(18)='TEMPERATURE [DEG C] '
                                                            : 1
CNAME(19)='SALINITY [PSS78]
                                                            : 0
CNAME(20)='SIO4 [(MOLES/LITER)*10**6] '
                                                            : 0
EOF1
#
    compile, link and run the plot program
#
case SDEVICE in
    tcolor | ecolor | SUNC | sunc | pscm1) cp $moddir/sec11.f secplo.f;;
                                   *) cp $moddir/sec11_bw.f secplo.f;;
esac
cft77 secplo.f
case SDEVICE in
    SU* | su*) segldr -o runplo2 secplo.o -lgksg -lncarg -lncarg_no calc mpaint oplib deflib ;;
           *) segldr -o runplo2 secplo.o -lgksg -lncarg -lncarg_no calc oplib deflib ;;
esac
runplo2
# result : gksm18.txt
cat PROTOK
cat GKS_ERROR
    Plot horizontal maps ("map11/map11_bw")
cat > MAPINP << EOF1
INPUT FILE FOR PLOTTING HORIZONTAL PATTERNS FROM OUTPUT OF CMODEL
TITLE='TEST'
LAYER(S) TO BE PLOTTED
                                                               : YES=1, NO=0
25 M LAYER 1
75 M LAYER 2
                                                               : 0
150 M LAYER 3
                                                               : 0
250 M LAYER 4
                                                               : 0
450 M LAYER 5
                                                               : 0
700 M LAYER 6
                                                               : 0
1000 M LAYER 7
                                                               : 0
2000 M LAYER 8
```

```
3000 M LAYER 9
                                                            : 0
4000 M LAYER10
                                                            : 0
5000 M LAYER11
                                                            : 0
                                                            : YES=1, NO=0
PARAMETER
CNAME(1)='TOTAL CO2 [(MOLES/LITER)*10**-6] '
                                                            : 0
                                                            : 0
CNAME(2)='ALKALINITY [(EQUIVALENTS/LITER)*10**-6] '
CNAME(3)='PHOSPHATE [(MOLES/LITER)*10**-6]
                                                            : 1
CNAME(4)='DISSOLVED OXYGEN [(MOLES/LITER)*10**-6] '
                                                            : 0
CNAME(5)=POC[(MOLES/LITER)*10**-6]
                                                            : 0
CNAME(6)='CALCITE [(MOLES/LITER)*10**-6] '
                                                            : 0
CNAME(7)='DELTA 13C
CNAME(8)='DELTA 14C
CNAME(9)='POC DELTA 13C'
                                                            : 0
CNAME(10)='POC DELTA 14C
CNAME(11)='CALCITE DELTA 13C'
CNAME(12)='CALCITE DELTA 14C'
CNAME(13)='DEGREE OF [CO3--] SATURATION (PERCENT) '
CNAME(14)='PH-VALUE
CNAME(15)='[CO3--] [(MOLES/LITER)*10**-6] '
CNAME(16)='SOLUBILITY PRODUCT
CNAME(17)='PREFORMED PO4 [(MOLES/LITER)*10**6] '
CNAME(18)='TEMPERATURE [DEG C] '
                                                            : 1
CNAME(19)='SALINITY [PSS78]
                                                            : 0
CNAME(20)='DISSOLVED GASEOUS CO2 (SURFACE) '
                                                            : 0
CNAME(21)='OCEAN-ATMOSPHERE DIFFERENCE IN PCO2 '
                                                            : 0
CNAME(22)='PRIMARY PRODUCTION [G/(M**2 MONTH)]
                                                            : 0
CNAME(23)='CALCITE PRODUCTION [G/(M**2 MONTH)]
                                                            : 0
CNAME(24)='ORG. C SEDIMENT POOL CONTENT [MOLE/M**2]': 0
CNAME(25)='CACO3 SEDIMENT POOL CONTENT [MOLE/M**2] ': 0
CNAME(26)='SIO4 [(MOLES/LITER)*10**6] '
CNAME(27)='NN
                                                            : 0
CNAME(28)='NN
                                                            : 0
CNAME(29)='NN
                                                            : 0
CNAME(30)='NN
                                                            : 0
EOF1
#
    compile, link and run the plot program
case $DEVICE in
    tcolor | ecolor | SUNC | sunc | pscm1) cp $moddir/map11.f mapplo.f;;
                                 *) cp $moddir/map11_bw.f mapplo.f;;
esac
cft77 mapplo.f
case $DEVICE in
    SU* | su*) segldr -o runplo3 mapplo.o -lgksg -lncarg -lncarg_no calc mpaint oplib deflib ;;
          *) segldr -o runplo3 mapplo.o -lgksg -lncarg -lncarg_no calc oplib deflib ;;
esac
runplo3
# result : gksm20.txt
cat PROTOK
cat GKS ERROR
set +e
```

```
pwd ls -l LLL="'ls | grep gksm'" for GKSFIL in $LLL do case $DEVICE in SUN | sun | SUNC | sunc) rcp $GKSFIL iceage:/home/k204002 ;; tcolor | ecolor | pscm1) spl f=$GKSFIL d=$DEVICE \ scale=18.9 p=/pf/m/m211021/perm/palettyn ;; psz1 | psm2) spl f=$GKSFIL d=$DEVICE scale=19.4 ;; versat) spl f=$GKSFIL d=$DEVICE scale=18.9;; esac done # exit
```

Appendix C PLOT OUTPUT EXAMPLES

In this section a subset of plots created by the **capost.job** shell script (see Appendix B) is shown.

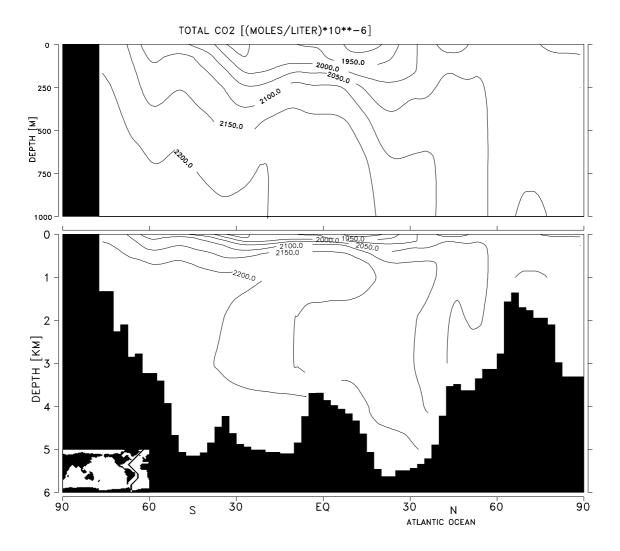


Figure 4 Example for a plot output showing the GEOSECS cross section of the Western Atlantic for the total CO_2 concentration [10^{-6} moles/liter].

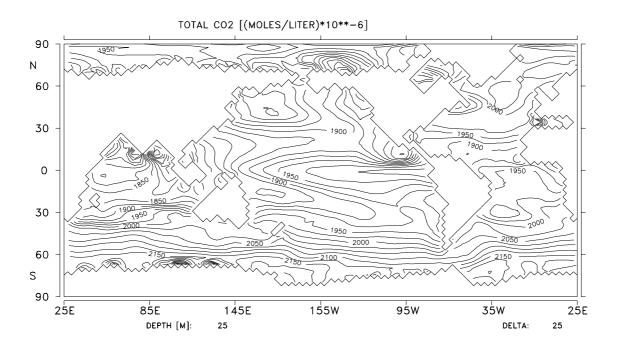


Figure 5 Example for a plot output showing the world map of the total CO_2 concentration [10^{-6} moles/liter] for a depth of 25 meters.

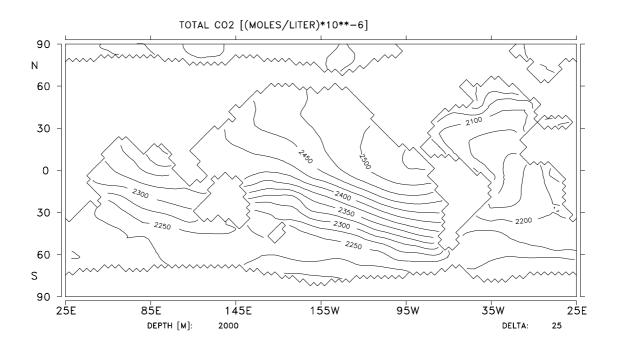


Figure 6 Example for a plot output showing the world map of the total CO_2 concentration [10^{-6} moles/liter] for a depth of 2000 meters.

Appendix D CODE NUMBERS USED BY POSTPROCESSING PACKAGE

Code	Quantity
1	¹² CO ₂
2	¹³ CO ₂
3	¹⁴ CO ₂
4	$\Sigma^{12}\mathrm{CO}_2$
5	total alkalinity
6	dissolved phosphate
7	dissolved oxygen
8	POC (12C)
9	CaCO ₃ (12C)
10	$\Sigma^{13}\mathrm{CO}_2$
11	$\Sigma^{14}\mathrm{CO}_2$
12	POC (13C)
13	POC (14C)
14	CaCO ₃ (¹³ C)
15	CaCO ₃ (14C)
16	pCO ₂ at the ocean surface
17	pCO ₂ (air) - pCO ₂ (water)
18	pH-value at the ocean surface
19	new production of POC
20	new production of CaCO ₃
21	POC (12C) sediment pool
22	CaCO ₃ (¹² C) sediment pool
23	depth at topography scalar points
24	CO ₃ supersaturation
25	PH-value
26	CO ₃ ²⁻ ion concentration
27	CaCO ₃ solubility product
28	preformed PO ₄
29	land/sea distribution
30	actual thickness at topography scalar points
31	zonal velocity component u
32	meridional velocity component v
33	potential temperature
34	salinity
35	depth at topography vector points
36	vertical velocity component w