Simple Shelf Sea Carbon Pump Model

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March 5, 2013

1 Introduction

The scope of this model is to test the contribution of particular biogeochemical mechanisms for to the seasonal shelf carbon pump, in particular non-Redfieldian processing of organic matter leading to carbon overconsumption. It is highly parameterised! As such it should probably be applicable to any shelf system, but parameter ranges are intended to represent the North Sea.

The model is written in R and designed to be run in large-number ensemble mode or as single model runs. Each run takes about 2 minutes on my old slow computer, or about 20 seconds on a node of the UEA cluster.

2 Model dimensionality, structure and boundary conditions

The model is a 1-dimensional (or maybe pseudo 1d) box model solved numerically by time-stepping. The model consists of a single box (the water column), which divides into a surface layer and bottom layer at the onset of 'spring'. There is no mixing or diffusion between these boxes until 'autumn' when tracers in the two boxes are mixed completely and a single-box arrangement continues for the rest of the year.

The inorganic carbon system is open to air-sea CO2 flux, allowing the model to take up or release carbon. Biological modifications to the carbon cycle are driven by nutrient (nitrogen). The model currently conserves carbon in the water column but (intentionaly, for simplicity) not nitrogen.

2.1 Boundary conditions

Boundary conditions that drive the model are listed in Table 1. Surface and bottom temperature, pCO2 in the atmosphere and wind speed are all represented by simple annual sine wave functions, defined by min and max values (in the case of temp and wind speed) or mean and amplitude (pCO2). Temperature is offset from a 1st Jan min/max so that its minimum occurrs later (some time in Feb is most realistic).

2.1.1 Driving the system: nitrate

At the onset of spring, the water column instantaneously stratifies and nitrate is drawn down to zero at a constant rate over SPRING_BLOOM_LENGTH (a largely pointless paramater on reflection, it could all just as well have happened

Boundary condition	controlling parameters
pCO2_atmos	AMPLITUDE, AVERAGE_pCO2 (μAtm)
temp (surface)	MIN_SURFACE_TEMP, MAX_SURFACE_TEMP (oC)
bottomtemp	MIN_BOTTOM_TEMP, MAX_BOTTOM_TEMP (oC)
wind	MIN_WIND, MAX_WIND (m/s)
nitrate	WINTER_NITRATE (μM)

Table 1: model boundary conditions

instantaneously...). However, it's not worth changing and it does make the model output look prettier! Once all that nitrate has gone, the spring bloom is over summer recycling begins and persists for SUMMER_LENGTH, at the end of which the whole water column is mixed and the model runs through the winter and ends immediately before the start of 'spring' in the following year.

2.1.2 Inorgnic carbon system

By default the model is initialised with the ocean and atmopshere at equilibrium with respect to CO_2, with DIC calculated from atmospheric pCO_2 and TA using the (T and S dependent) CO_2 system R package "seacarb" (http://cran.r-project.org/web/packages/seacarb/index.html). The model can be initialised out of equilibrium by specifying a non-zero value for the delta_pCO2 parameter (negative values representing supersaturation). DIC is taken up in Redfieldian proportions (Redfield ratio being a parameter of the model - i.e. not necessarily 6.6) with nitrate drawdown during the spring bloom, and in a fraction (TEP_fraction) of recycled production during summer. It is regenerated through remineralisation of organic matter in both surface and bottom layers. At each timestep pCO_2 is recalculated from DIC and TA (the latter is currently invariable but may in the future be modified by e.g. benthic alkalinity fluxes), and the flux calculated from pCO_2.

2.1.3 Organic material

Following the observations by our group (e.g. Suratman et al 2010, Johnson et al 2012) that a significant proportion (approx 50%) of winter nitrate is converted to semi-labile DON (slDON) which degrades slowly in the surface layer, the paramater nitrate_to_slDON_conv determines the proportion of drawn down nitrate which is transferred to DON, the remainder being exported instantaneously to the bottom layer as PON. POC is exported in Redfieldian proportions to PON, and semi-labile DOC (slDOC) is produced by default in Redfieldian proportions to slDON, but this can be controlled by the parameter slDOM_C_TO_N.

The controlling rate of summer recycling is the turnover of NH4 (NH4_turnover), which is reasonably well constrained and can be employed flexibly with better nitrogen schemes in the future. Carbon is turned over in Redfieldian proportions to the NH4, but a proportion of it is turned into TEP (transparent exopolymer particle carbon) via TEP_fraction, leading to new carbon fixation where otherwise there would be none.TEP has a very high C:N (or zero N in this model) and has been found to be produced under conditions of nutrient limitation, such as summer recycling, sometimes in large quantities.

Organic carbon is remineralised directly back to DIC. In the case of POC and slDOC, remineralisation is scaled to (per day) PON and slDON degradation rates (PONdeg, slDON_deg; for which values are available in the literature) using the POCdeg_factor and slDOC_deg_factor scaling parameters. TEP carbon is remineralised according to a per day rate (TEPdeg). All the degradation rates are subject to a 'Q10' temperature dependence, by default set to 2.

2.2 parameters and default values

All model parameters and their values in the default config are shown in Table 2. The choice of default parameter values and ranges used in ensemble runs are justified below.

2.2.1 Water column dimensions

Very little of the UK shelf is at a depth greater than 250m, in fact this depth approximated the top of the shelf break, based on bathymetric maps. Most of the shelf lies at around 100m, with the transition from tidally mixed to seasonally stratifying lying at approximately 40m. Thus in single box mode, depths are 10-40 (default 25) and in 2 box mode, 40-250 (default 100).

The mixed layer in the 2 box model has a default value of 50m with a possible range of 10-150m. SMLD is necessarily constrained by the minimum value of COLUMN_DEPTH, however.

2.3 Output variables

Table 2.3 lists the variables used in model calculations and recorded at each timestep for output.

2.4 Key model equations

Equations governing key processes are detailed here

2.4.1 air-sea CO2 flux

CO2 flux across the air-sea interface is calculated using the temperature and salinity dependent Henry's law constant function (KH_Molar_per_atmosphere) and water side transfer velocity (k_w) from the gas exchange scheme of Johnson 2010. k_w is calculated using the parameterisation of Nightingale et al 2000,

paramater	default value	description
RUN_NAME	n/a	name of run / experiment
out_dir	n/a	name of directoy to write run output into
MODE	2	mode 1 is for a non-stratifing water column and broken
SMLD	20m	surface mixed layer depth
COLUMN_DEPTH	100	whole water column depth
MIN_SURFACE_TEMP	4	
MAX_SURFACE_TEMP	16	
MIN_BOTTOM_TEMP	2	
MAX_BOTTOM_TEMP	8	
OFFSET	59	days from 1st Jan 'til temperature minimum
AVERAGE_pCO2	390 μatm	mean concentration from Weybourne observatory
AMPLITUDE	14 μatm	amplitude of annual pCO2 aWeybourne
MAX_WIND	7.2 m/s	
MIN_WIND	11.3	
WINTER_NITRATE	12 μM	
BLOOM_START_DAY	88 d	days from 1st Jan
BLOOM_DURATION	15 d	probably pointless, could set to 1
SUMMER_LENGTH	150 d	
init_TA	2300	value from Artioli et al 2012 for N. Sea
delta_pCO2	0	initialise with non-equilibrated CO2 (-ve val = ocean supersat)
NH4_turnover	0.25 μM/d	typical shelf sea ammonium turnover rate
TEP_fraction	0.2	fraction of summer C turnover going into TEP production
redfield	6.6	
slDOM_C_TO_N	redfield	C:N ratio of semi labile organic matter produced
nitrate_to_slDON_conv	0.5	proportion of spring bloom nitrate that goes into DON
slDON_deg	0.02 d^{-1}	degradation rate of semi labile DON
slDOC_deg_factor	0.5	rate of C remin is product of this and slDON deg rate
PONdeg	0.02 d^{-1}	rate of PON degradation
POCdeg_factor	0.5	as above
TEPdeg	0.005 d^{-1}	
Q10_REF_TEMP	15	deg rates used here are from about this temp
Q10	2	temp scaling of degradation rates

Table 2: parameter values for the default model config

	BOUNDARY CONDITIONS
day	model day
nitrate	nitrate 'envelope' generated by bloom_start day, bloom_duration and WINTER_NITRATE
pCO2_atmos	
temp	
bottomtemp	
wind	
dNO3	change in surface NO3 over time
	DIAGNOSTIC VARIABLES
pCO2	
DIC	
slDON	
slDOC	
airseaFlux	
deltapCO2	
TEPC	
PON	
POC	
BML_DIC	
BML_NO3	
total_C	total C in the whole water column

Table 3: model output

but is multiplied by a factor of 1.3 to approximately account for the difference between short term and long term averaged winds (i.e. non-linear k_w means long term average winds underestimate the significance of occasional high wind events on mean transfer. If anything this is likely to be an overestimate, causing the atmosphere-ocean system to equilibrate to a greater degree than in reality, which probably makes the carbon pump less efficient (more of the seasonally fixed carbon escapes back to the atmopshere the following winter).

```
calc_as_flux<-function(pCO2,pCO2_atmos,temp,wind){
deltapCO2<-KH_Molar_per_atmosphere("CO2",temp,S=35)*(pCO2_atmos-pCO2)*1e-6 #mol/l
    #1.3 scaling factor between short and long-term winds
k_w<-Nightingkw("CO2",temp,wind,35)*3600*24*1.3
flux<-1e6*deltapCO2*1000*k_w #umol/m2/day
flux
}
```

2.4.2 DIC uptake during the spring bloom

DIC is taken up during the spring bloom in Redfieldian proportions to the change in the nitrate concentration (a boundary condition of the model), dNO3.

```
 calc_DIC_uptake_from_NO3<-function(dNO3){
-dNO3*redfield
}
```

2.4.3 semi labile DOM production in surface layer

A proportion of nitrate taken up in each timestep is instantaneously transferred to semilabile DON

```
 calc_prod_slDON<-function(dNO3){
-dNO3*nitrate_to_slDON_conv
}
```

and carbon is transferred to the slDOC pool accordingly. Note that there is a structural bug in the code at the moment - the model only conserves carbon if slDOM_C_TO_N is equal to the redfield parameter (This is an easy fix - just replace DIC_uptake_from_nitrate with something a bit cleverer).

```
 calc_prod_slDOC<-function(dNO3){
calc_prod_slDON(dNO3)*slDOM_C_TO_N
}
```

2.4.4 POM flux to deep ocean

The remaining nitrogen which is taken up (dNO3*(1 - nitrate_to_slDON_conv)) and associated carbon (by Redfield) are instantaneously exported to the bottom layer

```
calc_PON_flux<-function(dNO3){
-dNO3*(1-nitrate_to_slDON_conv)*SMLD/BMLD
}

calc_POC_flux<-function(dNO3){
((-dNO3*redfield)-calc_prod_slDOC(dNO3))*SMLD/BMLD
}
```

2.4.5 TEP carbon production and export

A fraction of the carbon turned over by summer recyling production (determined from fixed ammonium turnover rate) is turned into TEP carbon during the summer period only. This TEP production draws down DIC in the surface but the TEP is instantaneously exported to depth.

```
 #calculate TEP production during summer period
calc_TEPC_prod<-function(timestep){
if(timestep > (BLOOM_START_DAY+BLOOM_DURATION) && timestep < mix_day){
NH4_turnover*redfield*TEP_fraction
} else {
0
}
}
```

2.4.6 Q10 rate scaling

A Q10 approach to scaling organic matter degradation rates is implemented, where Q10_REF_TEMP is the approximate temperature at which degradation rate measurements were made

```
 Q10_rate_scale<-function(temp){
Q10^((temp-Q10_REF_TEMP)/10)
}
```

2.4.7 Organic matter degradation rates

all organic matter is degraded by a simple first order rate function (i.e. d^{-1}), scaled to temperature by Q10.

```
 # semi-labile DON degradation in surface layer
 calc_slDON_deg<-function(slDON,temp){
slDON*slDON_deg*Q10_rate_scale(temp)
```

```
}

#semi-labile DOC degradation in surface layer
calc_slDOC_deg<-function(slDOC,temp){
slDOC*slDOC_deg*Q10_rate_scale(temp)
}

#PON degradation in bottom layer
calc_PON_deg<-function(PON,temp){
PON*PONdeg*Q10_rate_scale(temp)
}

#POC degradation in bottom layer
calc_POC_deg<-function(POC,temp){
POC*POCdeg*Q10_rate_scale(temp)
}


#TEP degradation rate in bottom layer
calc_TEPC_deg<-function(TEPC,temp){
TEPC*TEPdeg*Q10_rate_scale(temp)
}
```

2.5 what the model doesn't capture, but might in the future

Closed N cycle, ephemeral blooms, deep chlorophyll maximum, turbulent nutrient fluxes across thermocline, phosphorous!, variable surface mixed layer depth,benthic and riverine alkalinity fluxes, winter nutrient recharge, gradual breakdown in stratification, autumn blooms, microbial biomass, oxygen feedbacks with organic matter and benthic alkalinity

2.6 model implementation and operation

The model is written in R and is designed to run with config files, which overwrite default values from a default config file, which resides in the 'root' directory of the model.

2.6.1 code structure

where R files are denoted as "Rscript" they can be called from the command line and passed arguments to control their behaviour. They can then be included in bash scripts.

```
.
|-- core_model.R         # core model code
```

```
|-- intialise_model.R    # model initialisation called from core_model.R
|-- model_run.R          # Rscript to run a single instance of the model from a config
|-- experiment_run.R     # Rscript to run an ensemble experiment
|-- setup_experiment.R   # Rscipt to setup an ensemble experiment from a config file
|-- analyse_experiment.R # Rscript to parse experimet data and generate a .Rdata save
|-- eval_CO2_sys.R       # CO2 system parameter calculations
|-- K_calcs_Johnson_OS.R # Core model from Johnson (2010) for calculating H and kw
|-- compounds.dat        # compounds data file necessary for Johnson (2010) model
|-- sw_constituent_mass_fractions.dat # sw makeup data for Johnson (2010) model
|-- configs
|   |-- config files for single runs or experiments
|-- results
|   |-- results files from single runs
|-- experiments
|   |-- directories of results from ensemble experiments
```

2.6.2 config files

Model config files (e.g. default_config.R) are R files with a series of variable assigments, correspondind to parameters in the model, or run metadata. default_config.R provides default values (as listed in Table 2). Only non-default values need to be specified in experiment / run configs, from where they will 'overwrite' default values when the model is run.

e.g. a deeper-than-standard water column run

```
##################################################
### Deep water column run of default model #######
##################################################

## surface mixed layer depth
SMLD<-75

## water column depth
COLUMN_DEPTH<-250
```

'Run' config files contain single values of each parameter, allowing a single non-default run to be defined.'Experiment' config files allow a ranges of multiple parameter values to be explored in an experiment (either every permutation / combination) or by lhc sampling of the paramater ranges. In the below example, some parameters have a single, non-default value, some have a 3-member array and some a 10-member array. 10 is currently the hard-coded number of values per parameter in an ensemble experiment, each one can be specified (in a 10-member array), or the min and max values and distribution type (linear = 0, logarithmic =1) can be specified and the experiment setup script will do the rest...

```
#####################################################################
### Classic Refieldian LHC ensemble - everything happens at  ####
#### redfield, OM is instantaneously remineralised           ####
#####################################################################


RUN_NAME<-"classic_redfieldian_lhc"

out_dir<-RUN_NAME

#################################
##### WATER COLUMN DEPTHS   #####
#################################

## surface mixed layer depth
SMLD<-c(15,50,0)

## water column depth
COLUMN_DEPTH<-c(60,300,0)


#################################
###### BOUNDARY CONDITIONS  ######
#################################

## sine wave temperature variation defined from these values

MIN_SURFACE_TEMP<-c(0,5,0)
MAX_SURFACE_TEMP<-c(10,16,0)

OFFSET<-c(0,70,0)

AVERAGE_pCO2<-c(360,420,0)

AMPLITUDE<-c(0,20,0)

MIN_WIND<-c(6,9,0)
MAX_WIND<-c(9,12,0)
## model is initialised with winter nitrate and the bloom period is described by start day a

WINTER_NITRATE<-c(6,16,0) #uM
BLOOM_START_DAY<-88 #jday
BLOOM_DURATION<-15 #days

## summer length defines when the BML and SML are mixed into a single box again (they separa
```

```
SUMMER_LENGTH<-c(100,111,122,133,144,155,166,177,188,199) #days

## estimate of total alkalinity from artioli et al 2012
init_TA<-2300 #uM

## delta pCO2 defines starting disequilibium between atmos and surface ocean (+ve indicates
delta_pCO2<-0


###################################
######## PARAMETER VALUES ########
###################################

# ammonium turnover rate
NH4_turnover<-0 #uM day-1


## Proportion of spring bloom N turned into semi-labile DON
nitrate_to_slDON_conv<-0


#degradation rate of PON in BML


PONdeg<-0.8 #day-1
POCdeg_factor<-1


#"Q10" values for degradations
Q10<-1
```

2.6.3 setup scripts

A script (setup_experiment.R) is used to generate individual run config files and launch scripts (each to launch a chunk of the total ensemble runs sequentially, thus requiring fewer (longer) jobs to be submitted to a cluster) for an ensemble experiment defined by a single config file (see above).

The script can be run from the model home directory thus:

```
~/shelf-sea-carbon-pump-model$ Rscript setup_experiment.R classic_redfieldian_lhc 10000 100
```

The script takes three command line arguments: experiment_name, max_runs and chunk_size. It looks in the configs directory for the file named ¡experiment_name¿, parses the config file and generates a random lhc (using the ranges of varying parameter values in the config) of length max_runs (if the

number or permutations/combinations is less it will do all of them). It then writes out a config file for every run in the ensemble in the directory experiments/¡experiment_name¿ and ¡max_runs¿/¡chunk_size¿ number of shell script launch files, each of which submits a cluster job containing ¡chunk_size¿ runs to be solved sequentially. Gotchas: ¡max_runs¿/¡chunk_size¿ must be a whole number; if parameter values are specified in an array (rather than max,min,distribution type), there must the same number as the n_vals variable that is defined in the setup_experiment script. You have been warned.

2.7 model code

Model code is divided into two scripts. This is a hacky solution to parsing config files which are stored as .R files. I'm sure there's a better way of getting key-value pairs out of an ascii file into R than the very hack way I've done it (read the code if you fancy a laugh), but I haven't been able to find one!

core_model.R loads in external scripts and libraries (seacarb, K_calcs_Johnson_OS.R), plus the default config values; defines the functions which map to processes in the model (e.g. calc_slDON_deg) and other functions relating to evaluating amounts and concentrations of state variables at each timestep. It also contains the eval_timestep function which takes the current state of the model and the timestep index and moves the model forward by one timestep (i.e. day).

Finally it contains the model_run function, which initialises the model by calling initialise_model.R, constructs the output data frame and populates it by calling the eval_timestep function as many times as required. initialise_model.R takes config values to generate boundary conditions and creates a data frame of these values to be passed back to the core model code.

2.8 run scripts

model_run.R and experimet_run.R both run individual model runs, the former intended for standalone runs, the latter formembers of an ensemble, the main difference being the outdir being "results" in the former and "experimets/¡experiment_name¿" in the latter. model_run.R takes a single command line argument, ¡run_name¿, which is used to find the config file and to name the output file. experiment_run.R works in a similar way and is called from the 'chunk' shell scripts which will submit jobs to the UEA cluster, but could be easily modified for other purposes.

2.9 data processing scripts

The output of each model run is a csv file with one row per timestep and one column per output variable. Analyse experiment generates a data frame with one row per enseble member and one column per input parameter value, plus colums for net air-sea flux and the change in the total carbon inventory of the water column between the beginning and end of the run (these two parameters

should be equal if nothing's gone wrong...). This allows the broad scale investigation of the importance of parameter values on carbon uptake, although other digostic variables could be added in here.

2.10 Initial results

When run with the default config, there is net carbon uptake into the water column over the course of the seasonal cycle.

initial ensemble experiments (prior to implementing the overconsumption of carbon due to preferential remineralisation were configures as follows:

2.11 ensemble experiments

2.11.1 non-Redfieldian dynamics

2.11.2 TEP

TEP production has been found to be between 18 and 41 % of POC production in incubations of summer surface Baltic sea water by Engel2002. Thus we take a range of possible TEP production as a function of summer turnover to more-than cover this observed range, of 2 to 60 %.

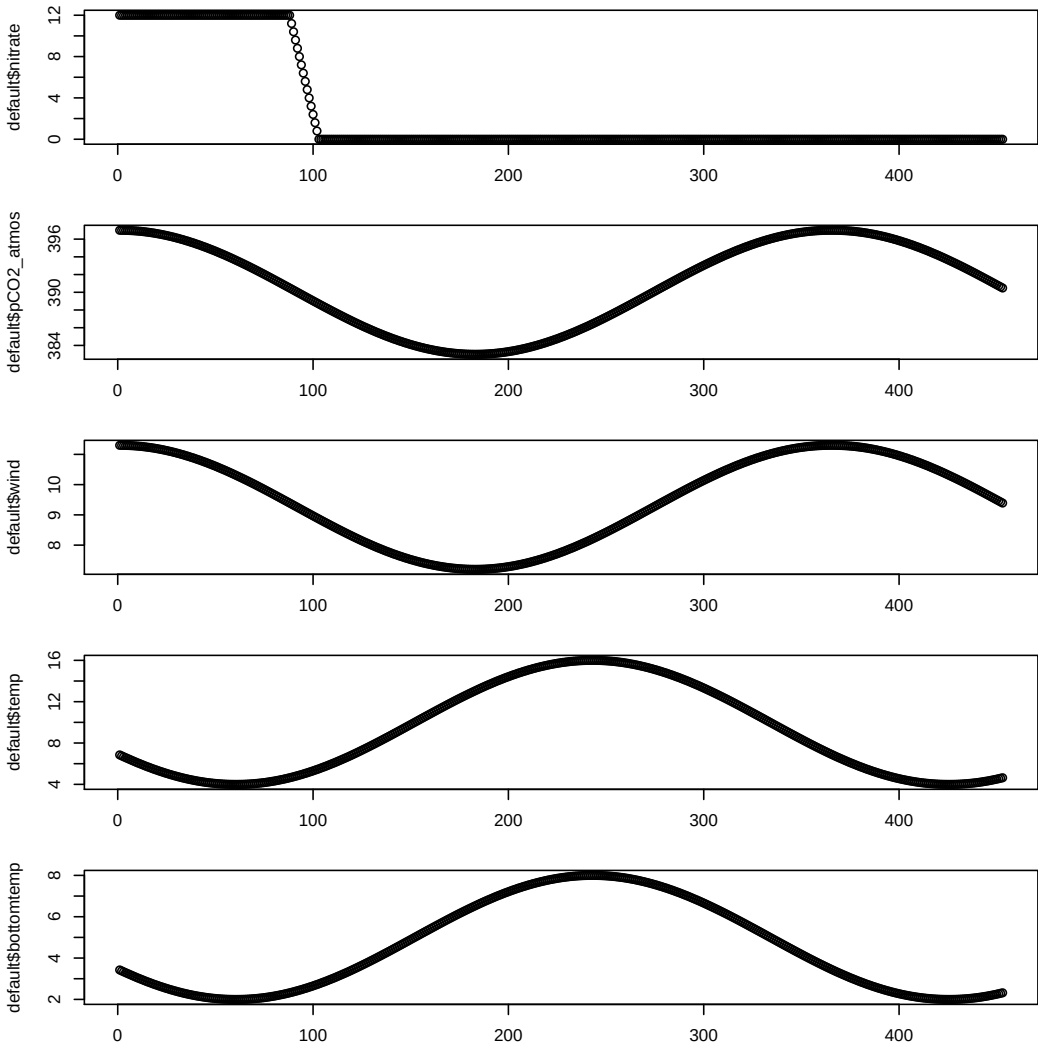

Figure 1: Boundary conditions in model default config

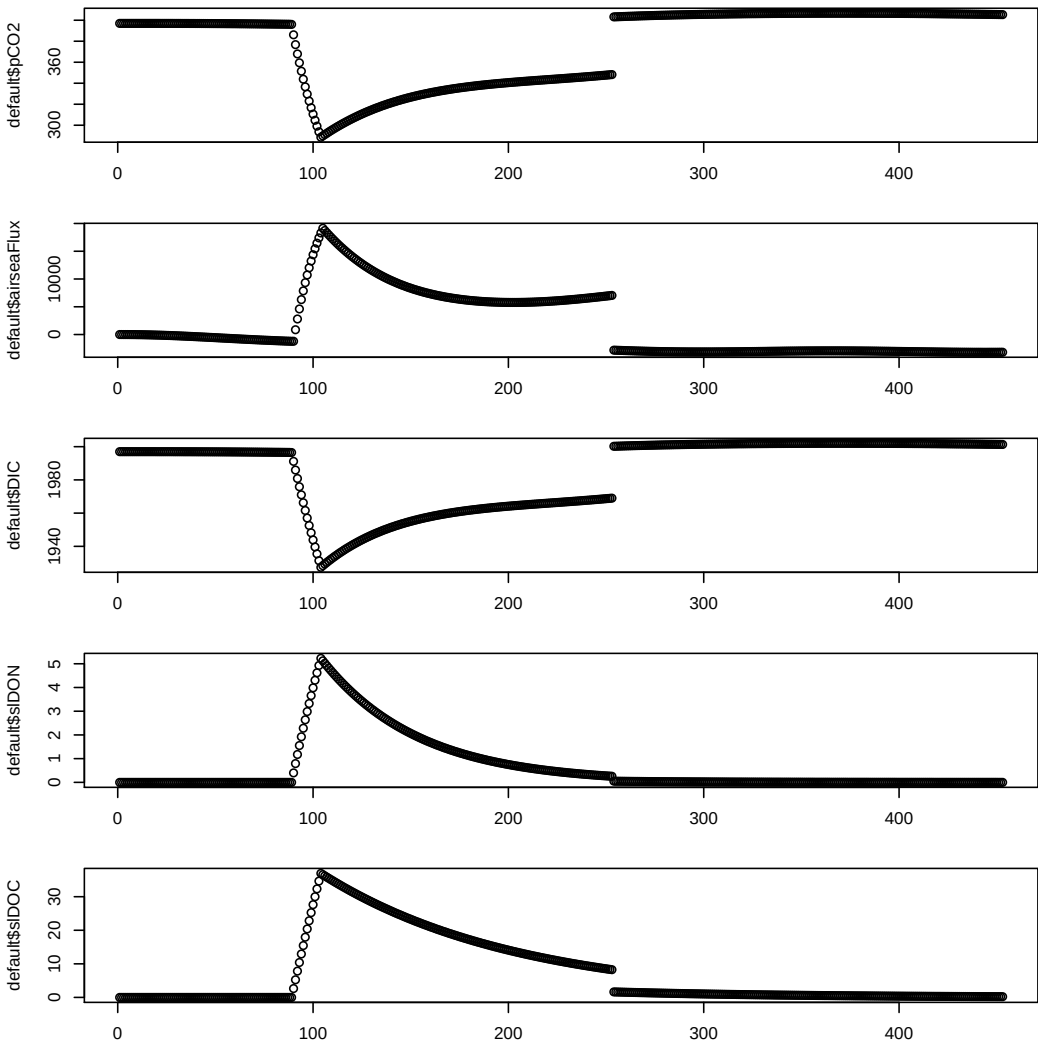

Figure 2: Results from model default config, surface parameters

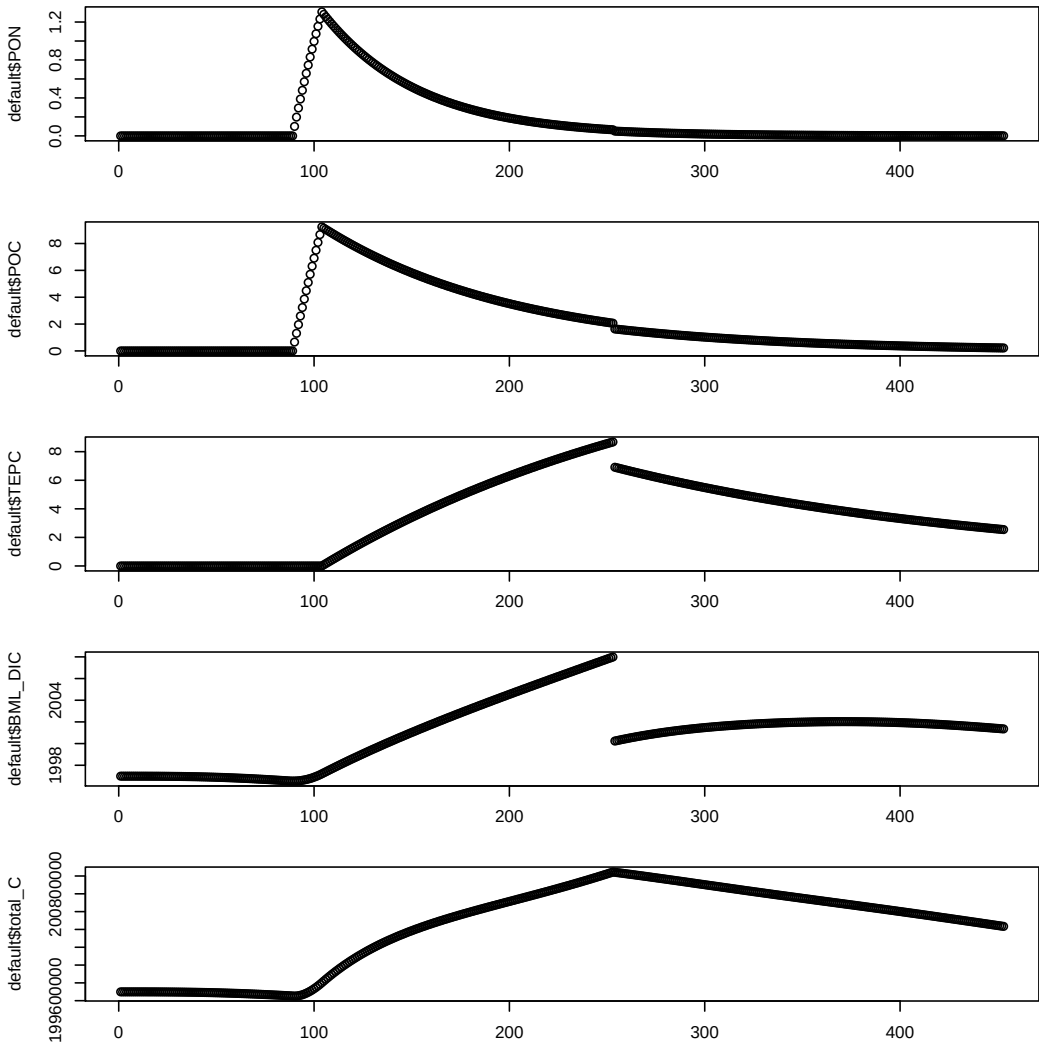

Figure 3: Results from model default config, BML parameters and total water column carbon

paramater	physical lhc	redfieldian lhc	deep lhc	shallow lhc
MODE	2	2	2	2
SMLD	c(15,50,0)	c (15,50,0)	c(20,60,0)	c(10,40,0)
COLUMN_DEPTH	c(60,300,0)	c(60,300,0)	250	50
MIN_SURFACE_TEMP	c(0,5,0)	c(0,5,0)	c(0,5,0)	c(0,5,0)
MAX_SURFACE_TEMP	c(10,16,0)	c(10,16,0)	c(10,16,0)	c(10,16,0)
MIN_BOTTOM_TEMP	c(-2,4,0)	c(-2,4,0)	c(-2,4,0)	c(-2,4,0)
MAX_BOTTOM_TEMP	c(6,10,0)	c(6,10,0)	c(6,10,0)	c(6,10,0)
OFFSET	c(0,70,0)	c(0,70,0)	c(0,70,0)	c(0,70,0)
AVERAGE_pCO2	c(360,420,0)	c(360,420,0)	c(360,420,0)	c(360,420,0)
AMPLITUDE	c(0,20,0)	c(0,20,0)	c(0,20,0)	c(0,20,0)
MAX_WIND	c(6,9,0)	c(6,9,0)	c(6,9,0)	c(6,9,0)
MIN_WIND	c(9,12,0)	c(9,12,0)	c(9,12,0)	c(9,12,0)
WINTER_NITRATE	0	c(6,16,0)	c(6,16,0)	c(6,16,0)
BLOOM_START_DAY	88	88	88	88
BLOOM_DURATION	15	15	15	15
SUMMER_LENGTH	c(100,111,122,133,144,155,166,177,188,199)	as phys	as phys	as phys
init_TA	c(2200,2400,0)	2300	2300	2300
delta_pCO2	c(-10,10,0)	0	0	0
NH4_turnover	0	0	0.25	0.25
TEP_fraction	0	0	c(0.02,0.6)	c(0.02,0.6)
redfield	6.6 (unused)	c(4,8,0)	6.6	6.6
slDOM_C_TO_N	redfield (unused)	redfield (unused)	c(4,10,0)	c(4,10,0)
nitrate_to_slDON_conv	0	0	c(0.1,0.8,0)	c(0.1,0.8,0)
slDON_deg	0.8 (unused)	0.8 (unused)	c(0.005,0.1,0)	c(0.005,0.1,0)
slDOC_deg_factor	1 (unused)	1 (unused)	c(0.1,1.1,0)	
PONdeg	0.8 (unused)	0.8	c(0.005,0.1,0)	c(0.005,0.1,0)
POCdeg_factor	1 (unused)	1	c(0.1,1.1,0)	c(0.1,1.1,0)
TEPdeg	1 (unused)	1(unused)	c(0.001,0.05,0)	c(0.001,0.05,0)
Q10_REF_TEMP	15	15	15	15
Q10	1 (unused)	1	c(1,4,0)	c(1,4,0)

Table 4: parameter values for the original (now defunct) ensemble experiments