Activation of the operational ecohydrodynamic model (3D CEMBS) – the ecosystem module*

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Abstract

The paper describes the ecohydrodynamic predictive model – the ecosystem module – for assessing the state of the Baltic marine environment and the Baltic ecosystem. The Baltic Sea model 3D CEMBS (the Coupled Ecosystem Model of the Baltic Sea) is based on the Community Earth System Model, which was adopted for

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the Baltic Sea as a coupled sea-ice-ecosystem model. The 3D CEMBS model uses: (i) hydrodynamic equations describing water movement, (ii) thermodynamic equations, (iii) equations describing the concentration distribution of chemical variables in the sea, and (iv) equations describing the exchange of matter between individual groups of organisms and their environment that make allowance for the kinetics of biochemical processes.

The ecosystem model consists of 11 main components: three classes of phytoplankton (small phytoplankton, large phytoplankton represented mainly by diatoms and summer species, mostly cyanobacteria) expressed in units of carbon and chlorophyll a as separate variables, zooplankton, pelagic detritus, dissolved oxygen and nutrients (nitrate, ammonium, phosphate and silicate). In operational mode, 48-hour atmospheric forecasts provided by the UM model from the Interdisciplinary Centre for Mathematical and Computational Modelling of Warsaw University (ICM) are used. All model forecasts are available on the website http://deep.iopan.gda.pl/CEMBaltic/new_lay/index.php. The results presented in this paper show that the 3D CEMBS model is operating correctly.

1. Introduction

The activity of organisms, which affects the circulation of matter and transformation of energy, has a major effect on the quality of the abiotic environment. Organisms modify their environment in a very short time: planktonic algae, for example, deplete resources of dissolved nutrients during the growing season. Thus, organisms interact not only with each other, but also with the abiotic environment. Populations in a biocoenosis[1] are connected with each other by a system of complicated interactions. Biocoenoses existing in a specific abiotic environment and interacting with its components form ecosystems. Defining the boundaries of an ecosystem is as difficult as defining the boundaries of a biocoenosis. Energy flows through the ecosystem, and matter circulates within the ecosystem. The flow of energy and matter through the ecosystem is not a real entity, but a factor that 'materializes' as a consequence of the accumulated activity of different organisms. A researcher who distinguishes trophic levels defines which pathways of energy and matter should be connected in order to form a picture of an ecosystem with a flux of energy and matter. Obviously, the functioning of an ecosystem can be explained by the general laws of physics and chemistry: the laws of thermodynamics, the law of conservation of mass, and the law of limited variability in biomass stoichiometry are of particular importance. These general laws permit a large number of alternative patterns in the energy and matter flow.

[1]A biocoenosis consists of plant and animal populations in a specific abiotic environment, interacting with each other via trophic relations.

Dzierzbicka-Głowacka and her co-workers have published several papers on hydrodynamic modelling (Dzierzbicka-Głowacka et al. 2011c, 2012d,e, 2013) and biological processes, for instance: Dzierzbicka-Głowacka (2000, 2005, 2006), Dzierzbicka-Głowacka et al. (2006, 2010a,b, 2011a,b, 2012b,c). In November 2012, the operational ecohydrodynamic model (3D CEMBS – new version) was launched at the Institute of Oceanology PAS on a 2 km grid with rivers, in a parallel version with the ecosystem module.

This paper presents the three-dimensional ecohydrodynamic model of the Baltic Sea 3D-CEMBS (3D Coupled Ecosystem Model Baltic Sea) – the ecosystem module, based on selected results of the model describing the functioning of the Baltic ecosystem. The 3D CEMBS model determines the spatio-temporal distributions of investigated pelagic variables for three classes of phytoplankton, nutrients (NO_3, NH_4, PO_4, SiO_3), zooplankton, dissolved oxygen and dissolved pelagic detritus, which are listed on the IO PAS website (http://deep.iopan.gda.pl/CEMBaltic/new_lay/index.php). The results given in this paper show that the 3D CEMBS model is operating correctly.

2. The 3D CEMBS model

2.1. Configuration

3D-CEMBS (3D Coupled Ecosystem Model of the Baltic Sea) is a coupled ice-ocean-ecosystem model consisting of five separate components, as well as an additional central coupler CPL7 that controls time, exchange of forces, domains, grids and other model data (see Figure 1). The model

Figure 1. 3D-CEMBS configuration

domain is the extended Baltic Sea. The ocean (POP model, version 2.1) and ice (CICE model, version 4.0) models are forced by the atmospheric data model (datm7). In addition, the river inflow of freshwater and nutrient deposition is processed by the land model (dlnd) (Dzierzbicka-Głowacka et al. 2012a,d, 2013).

The 3D CEMBS model can be briefly characterized as follows:

- It has a horizontal resolution of approximately 2 km (1/48°).
- The bathymetry (based on the ETOPO1 1 arc-minute global relief model) is represented by 21 vertical levels.
- The thickness of the first four surface layers is 5 metres.
- The model domain is based on stereographic coordinates with the equator in the centre of the Baltic Sea.
- The driver and coupling time step is 1440 seconds. The ocean model time step is 480 seconds (8 min).
- The POP modelled variables are temperature, salinity, currents and sea surface height.
- The CICE modelled variables are ice coverage and ice thickness.
- Data from 78 main rivers of the Baltic Sea are used to provide nutrient deposition from rivers (from Baltic Nest).
- Atmospheric nutrient deposition is obtained from HELCOM.
- 48 h atmospheric forcing data are taken from the ICM-UM model (University of Warsaw).

The ocean-ice model POPCICE for the Baltic Sea is described separately in Dzierzbicka-Głowacka et al. (2013).

2.2. Ecosystem model

Energy flows through an ecosystem in a unidirectional process and is gradually dispersed as it is consumed by organisms for their life functions, whereas matter circulates in an ecosystem and is constantly converted from the inorganic form into the organic one, and vice versa. Autotrophic organisms (phytoplankton) take up chemical elements and inorganic compounds dissolved in water (in the ionic form), which they use as building materials and energy, and then convert them into proteins, carbohydrates, lipids etc.

Heterotrophic consumers (zooplankton) feeding on both living (phytoplankton and smaller zooplankton) and dead organic matter (pelagic

detritus) produced at different trophic levels, use it to build up their bodies, but also remove it from their bodies as undigested food remains and products of metabolism (faeces, secretions). Microscopic organisms, mostly bacteria, decompose dead organic matter (plant and animal remains, and faeces) and transform it into simple inorganic compounds. The recovered nutrients (NO_3, NH_4, PO_4, SiO_3) are included in the next cycle of matter in the primary production process. The ecosystem model is based on an intermediate-complexity marine ecosystem model for the global domain (Moore et al. 2002) and consists of 13 main components: zooplankton, small phytoplankton, diatoms, cyanobacteria, one detrital class, dissolved oxygen and nutrients (nitrate, ammonium, phosphate and silicate). The class of small phytoplankton includes nano- and picophytoplankton, and can be inhibited by nitrates, phosphates and available light and temperature. The class of larger phytoplankton is represented by diatoms and is reduced by the aforementioned factors, as well as by silicates. The growth rate of cyanobacteria is determined by phosphates, temperature and light availability. The 3D CEMBS model has been adapted to allow for two nitrogen sources (ammonium and nitrate; nitrite was omitted from the model) as well as other nutrients like phosphorus or silicon. Nutrients may limit the growth of phytoplankton. Whichever nutrient has the lowest cell quota relative to the maximum quotas (the most limiting) modifies the carbon fixation rate. Nutrient inflows to the Baltic Sea are governed by the network of rivers (there are 78 in the current version of the model). Values of nutrient river deposition are taken from 'Baltic Nest' (MARE – Marine Research on Eutrophication, http://apps.nest.su.se/nest/) and of atmospheric deposition from HELCOM (http://www.helcom.fi/BSAP_assessment/ifs/ifs2011/en_GB/n_deposition/). There is only one zooplankton class (microzooplankton) in the 3D-CEMBS model, which grazes on the all three phytoplankton classes. Zooplankton growth rates vary with the food source: it is higher when small phytoplankton is the food source, and lower when diatoms are grazed. The detrital class mentioned above does not sink (SDetr/DOC), and thus represents dissolved organic carbon as well as very small particulates.

2.3. Model equations

In the 3D-CEMBS model, there is a second order advection-diffusion partial differential equation, similar to the conservation equations for temperature and salinity in the ocean model for each compartment in the ecosystem model. This equation describes the rate of change in the

concentration of the variables in time and space, taking the source and loss function into account (equation 1):

$$\frac{\partial S}{\partial t} + (V + w_s)\,\nabla S = \frac{\partial}{\partial z}\left(K_z \frac{\partial S}{\partial z}\right) + \sum_{j-1}^{2} \frac{\partial}{\partial x_i} + F_S\,, \tag{1}$$

where S is each model variable, V (u, v, w) is the velocity vector, w_s is the sinking velocity of pelagic detritus, K_z, K_{xi}, are vertical and horizontal turbulent diffusion coefficients and F_S is the biogeochemical source-sink term. The last term of equation (1) defines F_S, which describes possible sources and losses of the diffusing substance in the space being studied. F_S is determined from a knowledge of biogeochemical processes occurring in the marine environment and their mutual relations. These processes were selected from the relevant literature. The components of the flow velocity vector, temperature and salinity distributions were defined from the hydrodynamic module of the ocean-ice model POPCICE (Dzierzbicka-Głowacka et al. 2012a, 2013).

The model is based on relatively simple trophic interactions between variables. The structural relationships between different variables are presented in Figure 2. The equations for the individual variables are presented in Appendix A.

In 2013 it is planned to include in 3D CEMBS the large detrital pool (LDetr/POC) represented by particulate organic carbon.

2.4. Validation of the model

The preliminary validation of the model for the hydrodynamic module and the ecosystem module has been presented in two other papers (Dzierzbicka-Głowacka et al. 2012d, 2013).

The model results indicate that the pre-validated version describing KPP-parameterization and the long-term surface temperature distributions is operating correctly. The initial model validation of the main hydrodynamic parameters for 2000 is given in Dzierzbicka-Głowacka et al. (2013). The mean correlation coefficient for the sea surface temperature at four points was 0.97035 for 1963–2007. These results indicate excellent conformity of the newly adopted model, both with other models and with the experimental data. The results also show that the parameterization of horizontal mixing needs improvement (Dzierzbicka-Głowacka et al. 2013). This will be done in the next step of the work on the CEMBS model.

Figure 2. Structure of the ecosystem model

A relationship between the measurements of the main biogeochemical parameters and their calculated levels was obtained (Dzierzbicka-Głowacka et al. 2012d). The correlation coefficients for five selected points are presented in Dzierzbicka-Głowacka et al. (2012d – Table 1). The modelled values resembled the observed ones, with mean (for five points) correlation coefficients of 0.9634 for temperature, 0.9083 for nutrients, 0.6067 for chlorophyll *a*, 0.6189 for phytoplankton and 0.6404 for oxygen. The spatial and temporal variability of plankton is usually so great that any model with the right orders of magnitude in its outputs will fit the data. So even if the correlation coefficient is ca 0.6, this is still a good value.

2.5. Operational mode

The hydrodynamic and biological parts of the 3D CEMBS model work in the operational version and are available on the website (http://deep.iopan.gda.pl/CEMBaltic/new_lay/index.php). Every 6 hours, a 48 h forecast is generated based on the atmospheric forcing data provided by the UM-ICM model. It is possible to create forecast maps of the Baltic Sea for the following hydrodynamic parameters: temperature, salinity, currents, sea surface height, ice coverage and ice thickness, as well as biogeochemical

parameters – chlorophyll a concentration, phytoplankton and zooplankton biomasses, nutrient concentrations (NO_3, NH_4, PO_4, SiO_3) and dissolved oxygen concentration. The website enables the forecast area to be narrowed down according to the user's requirements. It is also possible to create graphs of temporal changes of these parameters at a given point. Moreover, an archive has been created for the period between 1 January 2012 and the date of the current state of the model, which allows changes in the environmental parameters of the Baltic Sea to be observed over a longer period of time (at present, a 1-day interval). The user selects the required time, variable, depth and area of a forecast.

The model works properly (see the website – Figure 3). The results of simulations for a 48 h forecast are presented for the model with a resolution of 2 km.

Figure 3. The selection page with the results of the 3D-CEMBS model

Forecast for the area:

- select the forecast time (48 h forecast) (Figure 4a),
- select the depth, one of the ten layers for which you would like to see the model results (Figure 4b),
- select a variable (chlorophyll a concentration, phytoplankton biomass, zooplankton biomass, nutrient concentration (NO_3, NH_4, PO_4, SiO_3), dissolved oxygen concentration) (Figure 4c),

Figure 4. Forecast for the area. Choose forecast parameters for 04.01.2013

- optionally you can set boundaries to narrow the area of interes by selecting two random points (corners of a rectangle) on the map (Figure 4d),
- to change the coordinates 'X' and 'Y' of selected points, press: 'Reset Coordinates' (Figure 4e),
- after all parameters have been selected, press: 'Submit' (Figure 4f).

Two examples are presented below for the following situations:
1. Forecast start: 08.08.2012, 00:00 UTC (Figure 5);
Select forecast parameters – hour: +24 (forecast is for 09.08.2012, 00:00 UTC), variable: phytoplankton [mmol C m^{-3}]; depth: 5–10 m (2nd layer), coordinate 'X': 265 to 502, coordinate 'Y': 125 to 321. After you have selected the parameters, press: 'Submit' and the screen will illustrate the results of the model.
2. Forecast start: 04.01.2013, 00:00 UTC (Figure 6);
Select forecast parameters – hour: +36 (forecast is for 05.01.2013, 12:00 UTC), variable: NO_3 concentration [mmol N m^{-3}]; depth: 20–26 (5th layer), coordinate 'X': 319 to 486, coordinate 'Y': 321 to 624. After you have selected the parameters, press: 'Submit' and the screen will illustrate the results of the model.

Figure 5. Forecast for the area. The example is for the following situation: select forecast parameters: hour: +24 (the forecast is for 2012.08.09, 00:00 UTC), variable: phytoplankton [mmol C m^{-3}]; depth: 5–10 m (2nd layer), coordinate 'X': 265 to 502, coordinate 'Y': 125 to 321

Figure 6. Forecast for the area. The example is for the following situation: select forecast parameters: hour: +36 (forecast is for 2013.01.05, 12:00 UTC), variable: NO_3 concentration [mmol N m^{-3}]; depth: 20–26 m (5th layer), coordinate 'X': 319 to 486, coordinate 'Y': 321 to 624

The user selection panel and a sample map with a forecast for chlorophyll *a* concentration (case 1) and NO_3 concentration (case 2) are illustrated in Figures 5 and 6 respectively.

3. Results of the 3D CEMBS model

This section gives some of the results obtained from the 3D CEMBS model and discusses the functioning of the Baltic ecosystem. The results presented below demonstrate that the model is operating correctly. Figure 7 lists the model results for hydrodynamic (temperature, salinity, water currents and water level) and biogeochemical variables (chlorophyll *a* concentration, biomass of phytoplankton and zooplankton, nutrient concentrations NO_3, NH_4, PO_4, SiO_4 and dissolved oxygen concentration) for 2 May 2012.

The rate of phytoplankton primary production in the growing season is usually very high. Owing to the short life span of these microscopic plants and the high productivity of the euphotic layer, phytoplankton is the main source of energy for other ecosystem elements, both in the open sea and in the coastal zone. Some phytoplankton is consumed directly by herbivorous zooplankton, but a large part of the phytoplankton sinks to the bottom.

Three phytoplankton abundance peaks are characteristic of the entire Baltic Sea; they are determined by the phenologies of the various groups of algae, which are associated with the environmental requirements of these plants. Regional differences, however, mostly in the water temperature, cause spring diatom blooms to appear already at the end of February in the Kattegat and the Belt Sea, between March and May in the Gdańsk Basin, but not before May in the Gotland Deep. The dates of the other peaks are more stable: the summer peak occurs between late July and early August, and the autumn one between late October and early November. Monthly distributions of the surface phytoplankton biomass for the 28th day of each month are presented in Figure 8. The area covered by spring algal blooms is usually the largest, whereas the extent of the autumn blooms is the least. In recent years, however, intense summer cyanobacterial blooms have become more and more frequent in different parts of the Baltic (Figure 9). Some of them, in contrast to other algae, may absorb nitrogen from the atmosphere, which enables them to develop even when the amount of nitrogen available from its water-soluble compounds is reduced during a hot summer (Figure 9). This phenomenon is particularly disturbing, because the cyanobacteria are represented by numerous toxic and potentially toxic species.

The phytoplankton biomass is determined from the calculated amount of organic carbon (C_{org}) contained in a cell, which takes a characteristic value in each group of algae; in the model this is expressed in mmol C m^{-3}. The concentration of chlorophyll *a* in the water is also used as an indicator of the biomass volume; in this model it is determined by separate equations for three classes of phytoplankton (see Appendix A).

Figure 7. Sample results for hydrodynamic and biogeochemical variables derived from the model 3D CEMBS for the whole Baltic Sea on 2 May 2012

Figure 8. Monthly surface phytoplankton biomass distributions for the 28th day of each month in 2012

Figure 9. Horizontal distributions of phytoplankton biomass and concentration of nutrient NO_3 for 31 July 2012

The water layer penetrated by light has a major effect on the existence of life in the sea, especially on plants, which use light energy to produce tissues and to maintain bodily functions. The amount of light available in the water column depends not only on the latitude, season and time of day, but increasingly also on the extent of water pollution in the sea area. An increase in the amount of organic matter, both suspended in the water and sinking to the bottom, as well as extensive and long-term phytoplankton blooms, reduce the depth of the euphotic zone. The transparency of Baltic Sea water is low. The maximum depth for photosynthesis is usually 20–30 m, although there are regions with no signs of vegetation just a few metres below the water surface.

Vertical distributions of pelagic variables are determined by the hydrological conditions prevailing in particular parts of the Baltic. Figure 10 illustrates the vertical distributions of phytoplankton biomass, nutrient (NO_3) concentrations, zooplankton biomass and dissolved oxygen concentration along transects AB (left) and CD (right) on 10 June 2012. Basically, the heated and less saline surface waters with a high phytoplankton biomass and lower nutrient concentrations are isolated from deeper waters, which are poor in plankton but rich in nutrients. Because the decomposition and mineralization of a large part of the matter take place mostly in deeper, benthic water layers and in the sediment, these environments constitute a reservoir of nutrients (Figure 10).

The zooplankton of the Baltic Sea is taxonomically poor. It consists mainly of crustaceans, rotifers, larval stages of fish, polychaetes,

Figure 10. Vertical distributions of phytoplankton biomass, nutrient concentrations, zooplankton biomass and dissolved oxygen concentration along transects AB (left) and CD (right) for 10 June 2012 (*continued on next page*)

Figure 10. (*continued*)

molluscs and protozoans. In the model it is represented by a one-state variable – microzooplankton – which is expressed in units of carbon [mmol C m^{-3}]. Depending on its sensitivity to light and its food preferences (herbivores stay closer to the sea surface), the zooplankton inhabits the water column to a depth at which its oxygen requirements are fulfilled (Figure 10).

Figure 11. Horizontal distribution of dissolved oxygen concentration at a depth of 135 m

The model also determines the concentration of dissolved oxygen, which decreases with depth (Figure 11). Deep waters with a low oxygen content (< 270 mmol O_2 m^{-3} in the central part of the Baltic at a depth of 135 m – Figure 11) serve as a continuously replenished store of variously degraded

organic matter, producing increasing amounts of hydrogen sulphide. The given value of O_2 is the average value for a layer of thickness 27 m; it may therefore have been overestimated in relation to the measured data, since the oxygen decrease in deeper regions is significant.

4. Conclusions

The marine ecosystem is a community of living organisms forming a biocoenosis together with all the elements of the inanimate environment.

Ecosystems are created by the animated part, i.e. relations with other organisms resulting from the coexistence of different categories of living organisms, which include producers, consumers and reducers. The inanimate part of the ecosystem is represented by the physical properties of the sea, such as the temperature, chemical composition and depth of the water, the type of bottom and the flow velocity. If we are talking about the Baltic Sea and abiotic factors having a major impact on the development of organisms, we cannot ignore the salinity, which acts as 'a masking factor'. When compared to deep-sea water regions, the low-salinity waters of the Baltic Sea are extremely poor in flora and fauna. At present, the salinity over most of the Baltic region ranges from 5 to 8 PSU, so the environment is too fresh for typical marine fauna and too saline for freshwater organisms. In the literature the 5–8 PSU range is often referred to as a 'minimum-species zone'. In almost all the seas of the world where one can observe the impact of fresh waters (estuaries, bays), the least number of species occurs within this range of salinity. This means that the Baltic is a unique, saltwater (brackish) sea doomed to low species diversity (Andrulewicz et al. 2008).

In the next step of our work, the 3D CEMBS model will be linked to the 3D population model for certain species of Baltic Copepoda (*Acartia* spp., *Pseudocalanus minutus elongatus* and *Temora longicornis*), which will permit the assessment of living resources and facilitate predictions of fishery yields. Food concentration and temperature are the factors that control the development of Copepoda in the Baltic Sea, while salinity is a limiting factor, in particular for the development of *Pseudocalanus minutus elongatus*.

The 3D CEBSM model is a three-dimensional model for the numerical simulation of the Baltic ecosystem, the concept of which was based on the solution used in the Community Earth System Model (CESM from NCAR – National Centre for Atmospheric Research) and activation of the interaction between three main modules, the ice model, the hydrodynamic model and the biochemical model. The ocean-ice module of the 3D CEMBS model was activated in the operational system on the server of the Institute of Oceanology PAS (http://deep.iopan.gda.pl/CEMBaltic/new_lay/index.

php) in March 2012, and the ecosystem module for biochemical variables in November 2012. The model operates on the basis of meteorological data: 2 m air temperature and specific humidity, sea level pressure, precipitation (rain and snow), short- and long-wave downward radiation, wind speed at 10 m height and air density. The operational mode uses 48 h atmospheric forecasts provided by the UM model from the Interdisciplinary Centre for Mathematical and Computational Modelling of Warsaw University (ICM).

The 3D CEMBS model of the Baltic ecosystem consists of:

- the CICE ice model describing the ice coverage and ice thickness;
- the hydrodynamic POP module describing the distributions of temperature, salinity, currents and sea level;
- the biochemical model describing (i) selected groups of organisms (three classes of phytoplankton, and zooplankton as one class) and chemical variables (oxygen, nutrients (for NO_3, NH_4, PO_4 and SiO_3), as well as dissolved pelagic detritus) and (ii) quantitative changes in the biomass of selected groups of organisms as a result of their interactions and the impact of external conditions (abiotic variables).

The variables presented on the website for a 48 h forecast are hydrodynamic (temperature, salinity, currents, sea surface height, ice coverage and ice thickness) and biochemical variables (biomass of phytoplankton and zooplankton, chlorophyll *a* concentration, dissolved oxygen concentration, concentrations of nutrients (NO_3, NH_4, PO_4, SiO_3) and concentration of dissolved pelagic detritus).

The application of the proposed numerical method enables real-time monitoring and evaluation of the Baltic Sea environment as an inland sea characterized by high biological productivity and particularly threatened by the effects of economic development.

In the next step, we plan to activate an operational system of the model, including assimilation of the satellite data within the SatBałtyk project (Woźniak et al. 2011a,b) (to be presented in a separate paper). In temperate latitudes, the amount of data on sea colour is limited by clouds, so satellite data assimilation models are an important part of the SatBałtyk project (the current model included).

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Appendix A

Ecosystem variables

$Phyt_{sp}C$	small phytoplankton carbon [mmol C m^{-3}]
$Phyt_{sp}Chl$	small phytoplankton chlorophyll [mg Chl m^{-3}]
$Phyt_{diat}C$	diatom carbon [mmol C m^{-3}]
$Phyt_{diat}Chl$	diatom chlorophyll [mg Chl m^{-3}]
$Phyt_{diaz}C$	cyanobacteria carbon [mmol C m^{-3}]
$Phyt_{diaz}Chl$	cyanobacteria chlorophyll [mg Chl m^{-3}]
$zooC$	zooplankton carbon [mmol C m^{-3}]
PO_4	dissolved inorganic phosphate [mmol P m^{-3}]
NO_3	dissolved inorganic nitrate [mmol N m^{-3}]
SiO_3	dissolved inorganic silicate [mmol Si m^{-3}]
NH_4	dissolved ammonia [mmol N m^{-3}]
O_2	dissolved oxygen [mmol O m^{-3}]
$SDetr$	dissolved pelagic detritus [mmol C m^{-3}]

Calibration coefficients for phytoplankton and zooplankton

Coefficient	Small phyto-plankton ($i = sp$)	Diatom ($i =$ diat)	Cyano-bacteria ($i =$ diaz)	Unit	Description
PC_{ref}	9.40	9.40	2.50	day^{-1}	maximum carbon-specific rate at T_o
kNO_3	0.25	0.50	–	mmol N m^{-3}	nitrate half saturation coefficient
kNH_4	0.25	0.50	–	mmol N m^{-3}	ammonium half saturation coefficient
kPO_4	0.05	0.10	0.50	mmol P m^3	phosphate uptake
$kSiO_3$	–	0.25	–	mmol Si m^3	silicate half saturation coefficient
$alphaChl$	0.34	0.30	0.17	mmol C m^2 mg^{-1} Chl W sec	initial slope of P_I curve
$u$max	2.50	1.95	0.90	day^{-1}	maximum zooplankton growth rate at T_0
$zgrz$	1.00	0.70	1.00	mmol C m^{-3}	grazing coefficient
$zingest$	0.30	0.30	0.21	–	zooplankton ingestion coefficient
$lossthres$	0.001	0.02	0.01	mmol C m^{-3}	concentration where losses approach zero
$mort$	0.15	0.15	0.17	day^{-1}	mortality rate

Calibration coefficients for phytoplankton and zooplankton (*continued*)

Coefficient	Small phyto-plankton ($i = sp$)	Diatom ($i =$ diat)	Cyano-bacteria ($i =$ diaz)	Unit	Description
$mort2$	0.0035	0.0035	0.00	$\mathrm{day}^{-1}\ (\mathrm{mmol\,C\ m}^{-3})^{-1}$	quadratic mortality rate
$aggratemax$	0.75	0.75	0.00	day^{-1}	maximum aggregation rate
$thetaNmax$	2.50	4.00	2.50	$\mathrm{mg\,Chl\ mmol}^{-1}\ \mathrm{N}$	maximum theta N
$parmdetr$	0.10	0.25	0.10	–	fraction of zooplankton losses to detrital pool when different kinds of phytoplankton are eaten

Other calibration coefficients

Coefficient	Value	Unit	Description
Q	0.137	$\mathrm{mmol\,N/mmol\,C}$	N/C ratio of phytoplankton and zooplankton
Qp	0.00855	$\mathrm{mmol\,P/mmol\,C}$	P/C ratio of phytoplankton
$Qpdiaz$	0.002735	$\mathrm{mmol\,P/mmol\,C}$	cyanobacteria P/C ratio
Qsi	0.137	$\mathrm{mmol\,Si/mmol\,C}$	diatom initial silicate/carbon ratio
$kappanitrif$	0.06	day^{-1}	nitrification inverse time constant
$parlim$	5.0	$\mathrm{W\ m}^{-2}$	PAR limit for nitrification
$zmort$	0.08	$\mathrm{day}^{-1}\ (\mathrm{mmol\,C\ m}^{-3})^{-1}$	zooplankton linear mortality rate
$zmort2$	0.42	$\mathrm{day}^{-1}\ (\mathrm{mmol\,C\ m}^{-3})^{-1}$	quadratic zooplankton linear rate
$lossthreszoo$	0.2	$\mathrm{mmol\,C\ m}^{-3}$	zooplankton concentration where losses approach zero
$kchl$	$0.03\ 10^{-2}$	$\mathrm{cm}^{-1}\ (\mathrm{mg\,Chl\ m}^{-3})^{-1}$	attenuation chlorophyll coefficient for PAR
kh_2o	$0.15\ 10^{-2}$	cm^{-1}	attenuation H_2O coefficient for PAR
$denitrifCN$	0.854	–	carbon:nitrogen ratio for denitrification
$rNfixphoto$	1.3335	–	N fixation relative to C fixation
$labileratio$	0.65	–	fraction of losses to DOC routed directly to DIC

Other calibration coefficients (*continued*)

Coefficient	Value	Unit	Description
diatlossdc	0.99	–	fraction of diatom loss to DOC
grazespdic	0.30	–	fraction of small phytoplankton grazing to DIC
grazediatdic	0.10	–	fraction of diatom grazing to DIC
grazediazdic	0.44	–	fraction of cyanobacteria grazing to DIC
grazediazzoo	0.21	–	fraction of cyanobacteria grazing to zooplankton
grazesiremin	0.33	–	fraction of diatom Si grazing that is remineralized
grazespdoc	0.40	–	fraction of small phytoplankton grazing to DOC
grazediatdoc	0.35	–	fraction of diatom grazing to DOC
grazediazdoc	0.35	–	fraction of cyanobacteria grazing to DOC
reminDOM	0.00667	day^{-1}	detritus remineralization rate
dcO_2	0.688	–	Redfield ratio carbon:oxygen
$diazdcO_2$	0.780	–	Redfield ratio carbon:oxygen for cyanobacteria
dcO_2remin	0.848	–	Redfield ratio remineralization carbon:oxygen

3D-CEMBS ecological model equations

Phytoplankton:

Change in phytoplankton biomass:

$$\frac{d(Phyt_iC)}{dt} = photo_iC - graze_i - loss_i - agg_i\,,$$

$$\frac{d(Phyt_iChl)}{dt} = photoacc_i - thetaC_i\ (graze_i + loss_i + agg_i)\,,$$

$$(i = sp,\ diat,\ diaz)\,,$$

where $Phyt_iC$ – small phytoplankton/diatom/cyanobacteria carbon concentration [mmol C m^{-3}], $Phyt_iChl$ – small phytoplankton/diatom/cyanobacteria Chl concentration [mg Chl m^{-3}], $photoC_i$ – carbon-fixation

[mmol C m^{-3} sec^{-1}], $graze_i$ – grazing rate [mmol C m^{-3} sec^{-1}], $lossi_i$ – non-grazing mortality [mmol C m^{-3} sec^{-1}], agg_i – aggregation loss [mmol C m^{-3} sec^{-1}], $photoacc_i$ – chlorophyll synth. term in photoadaptation [mg Chl m^{-3} sec^{-1}], $thetaC_i$ – small phyt/diatom/cyanobacteria local Chl/C ratio [mg Chl /mmol C].

Primary production factors:

$$photoC_i = PCphoto_i \; Phyt_iC \,,$$

$$PCphoto_i = PC\max_i \; lightlim_i \,,$$

$$PC\max_i = PCref_i \; nut(i) \; Tfunc \qquad (i = sp,\, diat,\, diaz) \,,$$

$$photoacc_i = \frac{pChl_i \; PCphoto_i \; Q}{thetaC_i} \; Phyt_iChl \,,$$

$$pChl_i = \frac{thetaN\max \; PCphoto_i}{alphaChl_i \; thetaC_i \; PARavg} \,,$$

$$thetaC_i = \frac{Phyt_iChl}{Phyt_iC} \,.$$

Nutrient limitation factor:

$$nut(sp) = \min(VNtot, VPO_4) \,,$$

$$nut(diat) = \min(VNtot, VPO_4, VSiO_3) \,,$$

$$nut(diaz) = VPO_4 \,.$$

- nutrient uptake rates:

$$VNO_3 = \frac{\dfrac{NO_3}{kNO_3}}{1 + \dfrac{NO_3}{kNO_3} + \dfrac{NH_4}{kNH_4}} \,,$$

$$VNH_4 = \frac{\dfrac{NH_4}{kNH_4}}{1 + \dfrac{NO_3}{kNO_3} + \dfrac{NH_4}{kNH_4}} \,,$$

$$VNtot = VNO_3 + VNH_4\,,$$

$$VPO_4 = \frac{PO_4}{PO_4 + kPO_4}\,,$$

$$VSiO_3 = \frac{SiO_3}{SiO_3 + kSiO_3}\,.$$

:

$$lightlim_i = 1 - exp\left(\frac{-alphaChl_i\ thetaC_i\ PARavg}{PC\max_i}\right),$$

$$PARavg = \frac{0.45\,PAR\ e^{(-KPARdz)}\ \left(1 - e^{(-KPARdz)}\right)}{KPARdz}\,,$$

$$KPARdz = \left(kchl\ \sum Phyt_iChl + kh_2o\right)\ dz(k)\,,$$

where PAR – incoming solar radiation [W m^{-2}], $PARavg$ – average PAR over mixed layer depth [W m^{-2}], $KPARdz$ – PAR adsorption coeffiecent (non-dim), $dz(k)$ – thickness of layer k [cm] .

Phytoplankton grazing and losses:

$$graze_i = u\max_i\ zooC\ \frac{{Pprime_i}^2}{{Pprime_i}^2 + zgrz_i}\ Tfunc\,,$$

$$Pprime_i = PhycC_i - lossthres_i\,,$$

$$loss_i = mort_i\ Pprime_i\ Tfunc\,,$$

$$agg_i = \min\left(aggratemax_i\ Pprime_i;\ mort2_i\ {Pprime_i}^2\right).$$

Temperature response function (T in °C):

$$Tfunct = 2^{\frac{(T+273.16)-(T_o+273.16)}{10}}\,.$$

Nutrients:

- nitrate NO_3

$$\frac{d(NO_3)}{dt} = NITRIF - DENITRIF - \sum_i upNO_{3i}\,,$$

where $NITRIF$ – nitrification ($NH_4 \rightarrow NO_3$) [mmol N m^{-3} sec^{-1}], $DENITRIF$ – denitrification ($NO_3 \rightarrow N_2$) [mmol N m^{-3} sec^{-1}], $\sum upNO_{3i}$ – nitrate uptake by small phytoplankton + diatoms + cyanobacteria [mmol N m^{-3} sec^{-1}].

$$NITRIF = \begin{cases} kappanitrif \;\; NH_4 & PARout < parlim \\ \dfrac{\log\left(\dfrac{PARout}{parlim}\right)}{-KPARdz} & PARin < parlim \end{cases},$$

$$DENITRIF = \frac{r\text{emin}DOC}{denitrifCN},$$

$$\sum_i upNO_{3i} = Q \;\; \frac{VNO_3}{VNtot} \;\; photo_iC\,.$$

- ammonium NH_4

$$\frac{d(NH_4)}{dt} = Q \;\; (lossDICsp + lossDICdiat + lossDICdiaz + \\ + lossDICzoo + grazeDICsp + grazeDICdiat + \\ + grazeDICdiaz) + r\text{emin}DON + diazNexcrete + \\ - NITRIF - \sum_i upNH_{4i},$$

where $\sum upNH_{4i}$ – ammonium uptake by small phytoplankton + diatoms + cyanobacteria [mmol N m^{-3} sec^{-1}], $lossDIC$ – non-grazing mortality of phytoplankton/zooplankton routed to DIC [mmol C m^{-3} sec^{-1}], $grazeDIC$ – grazing rate on phytoplankton routed to DIC [mmol C m^{-3} sec^{-1}], $reminDON$ – portion of DON remineralized [mmol N m^{-3} sec^{-1}], $diazNexcrete$ – cyanobacteria fixed nitrogen excretion [mmol N m^{-3} sec^{-1}].

$$lossDICsp = labileratio \;\; loss(sp),$$
$$lossDICdiat = diatlossdc \;\; labileratio \;\; loss(diat),$$
$$lossDICdiaz = labileratio \;\; loss(diaz),$$
$$lossDICzoo = labileratio \;\; zooloss \; (1 - zoodetr),$$
$$grazeDICsp = grazespdic \;\; graze(sp),$$
$$grazeDICdiat = grazeditdic \;\; graze(diat),$$

$$grazeDICdiaz = grazediaz\ graze(diaz)\,,$$

$$remin DON = DON\ reminDOM\,,$$

$$\sum_i upNH_{4i} = Q\ \frac{VNH_4}{VNtot}\ phto_iC\,,$$

$$diazNexcrete = Q\ photoC(diaz)\ (rNfixphto - 1)\,.$$

- phosphate PO_4

$$\frac{d(PO_4)}{dt} = Qp\ \ (lossDICsp + lossDICdiat + lossDICzoo +$$
$$+ grazeDICsp + grazeDICdiat + pchotoC(diat)) +$$
$$+ remin DOP + lossDIPdiaz - upPO_4sp - upPO_4diaz\,,$$

where $reminDOP$ – portion of DOP remineralized [mmol P m^{-3} sec^{-1}], $lossDIP$ – phosphate from mortality routed to remineralization [mmol P m^{-3} sec^{-1}], $upPO_4sp/diaz$ – phosphate uptake by small phytoplankton/cyanobacteria [mmol P m^{-3} sec^{-1}].

$$remin DOP = DOP\ reminDOM\,,$$

$$upPO_4sp = photoC(sp)\ Qp\,,$$

$$upPO_4diaz = photoC(diaz)\ Qpdiaz\,,$$

$$lossDIPdiaz = labileratio\ Qpdiaz\ (graze(diaz) + loss(diaz)) +$$
$$- Qp\ (grazePOCdiaz + grazezoo(diaz))\,.$$

- dissolved SiO_3

$$\frac{d(SiO_3)}{dt} = Qsi\ (grazesiremin\ graze(diat) +$$
$$+ diatlossdc\ loss(diat)) - upSIdiat\,,$$

where $upSIdiat$ – silicon uptake by diatoms [mmol Si m^{-3} sec^{-1}],

$$upSIdiat = Qsi\ photoC(diat)\,.$$

Detritus (SDetr) and zooplankton:

$$\frac{d(SDetr)}{dt} = lossDOCdiat + lossDOCdiaz + lossDOCzoo +$$

$$+ grazeDOCsp + grazeDOCdiat + grazeDOCdiaz +$$

$$- reminDOC\,,$$

$$\frac{d(zooC)}{dt} = grazezoo - zooloss\,,$$

where $zoodetr$ – fraction of zooplankton losses into detritus pool (non-dim), $zooloss$ – mortality and higher trophic grazing on zooplankton [mmol C m^{-3} sec^{-1}], $grazezoo$ – grazing on phytoplankton routed to zooC [mmol C m^{-3} sec^{-1}], $reminDOC$ – remineralization of SDetr/DOC [mmol C m^{-3} sec^{-1}].

$$lossDOCdiat = (1 - labileratio)\ \ diatlossdc\ \ loss(diat)\,,$$
$$lossDOCdiaz = (1 - labileratio)\ \ loss(diaz)\,,$$
$$lossDOCzoo = (1 - labileratio)\ \ zooloss\ (1 - zoodetr)\,,$$
$$grazeDOC(sp) = grazespDOC\ \ graze(sp)\,,$$
$$grazeDOC(diat) = grazediatDOC\ \ graze(diat)\,,$$
$$grazeDOC(diaz) = grazediatDOC\ \ graze(diaz)\,,$$
$$reminDOC = SDetr\ \ reminDOM\,,$$
$$grazezoo(sp) = zingest\ \ graze(sp)\,,$$
$$grazezoo(diat) = zingest\ \ graze(diat)\,,$$
$$grazezoo(diaz) = grazdiazzoo + graze(diaz)\,,$$
$$grazezoo = \sum(grazezoo(sp) + grazezoo(diat) +$$
$$+ grazezoo(diaz))\,,$$
$$zooloss = (zmort2\ Zprime^{1.4} + zmort\ Zprime)\ Tfunc\,,$$
$$Zprime = zooC - lossthres\ \ lossthreszoo\,,$$
$$zooDetr = \frac{\sum_{phyt1}^{phyt3}(paramDetr\ graze)}{\sum_{phyt1}^{phyt3} graze + 3}\,.$$

Dissolved oxygen:

$$\frac{d(O_2)}{dt} = O_2prod - O_2con\,,$$

where O_2prod – oxygen production [mmol m^{-3} sec^{-1}], O_2con – oxygen consumption [mmol m^{-3} sec^{-1}], $diazNfix$ – cyanobacteria total nitrogen fixation [mmol N m^{-3} sec^{-1}].

$$O_2prod = O_2prod(sp) + O_2prod(diat) + O_2prod(diaz)\,,$$

$$O_2prod(sp) = photoC(sp)\ \left(\frac{upNO_3sp}{(upNO_3sp + upNH_4sp)\ dcO_2}\ + \right.$$

$$\left. + \frac{upNH_4sp}{(upNO_3sp + upNH_4sp)\ dcO_2remin}\right)\,,$$

$$O_2prod(diat) = photoC(diat) \times$$

$$\times \left(\frac{upNO_3diat}{(upNO_3diat + upNH_4diat)\ dcO_2}\ + \right.$$

$$\left. + \frac{upNH_4diat}{(upNO_3diat + upNH_4diat)\ \ dcO_2remin}\right)\,,$$

$$O_2prod(diaz) = photoC(diaz)\ \times$$

$$\times \left(\frac{upNO_3diaz}{(upNO_3diaz + upNH_4diaz + diazNfix)\ dcO_2} + \right.$$

$$+ \frac{upNH_4diaz}{(upNO_3diaz + upNH_4diaz + diazNfix)\ dcO_2remin} +$$

$$\left. + \frac{diazNfix}{(upNO_3diaz + upNH_4diaz)\ diazdcO_2}\right)\,,$$

$$diazNfix = Q\ photoC(diaz)\ rNfixphoto - upNO_3diaz +$$

$$- upNH_4diaz\,,$$

$$O_2con = \frac{1}{dcO_2remin} \; (lossDICsp + lossDICdiat +$$

$$+ lossDICdiaz + lossDICzoo + grazeDICsp +$$

$$+ grazeDICdiat + grazeDICdiaz + reminDOC) +$$

$$+ 2 \; NITRIF \, .$$