

ANNEX 3

Models included in the catalogue: a short description

Dissemination level

**Restricted to other programme participants
(including the Commission Services)**

LEAD CONTRACTOR

JRC- JOINT RESEARCH CENTRE, EUROPEAN COMMISSION

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Contents

1.	Hydrodynamic models	1
1.1.	ROMS	1
1.2.	POM	2
1.3.	NEMO.....	2
1.4.	GETM-GOTM	3
1.5.	POLCOMS	4
1.6.	MOHID	4
2.	Biogeochemical models	5
2.1.	N ₂ P ₂ Z ₂ D ₂	5
2.2.	ERSEM	5
2.3.	BFM	7
2.4.	ECOSMO	8
2.5.	LIFE: Pelagic Biogeochemical Model	9
2.6.	ERGOM-MOM and ERGOM-Fish, the Ecological ReGional Ocean Model	10
2.7.	BIMS-ECO	12
2.8.	BALTSEM, the Baltic Sea Long-Term large-Scale Eutrophication Model	13
2.9.	SPBEM St. Petersburg Eutrophication Model	14
2.10.	BiOEBUS Eastern Boundary Upwelling Systems.....	15
2.11.	RCO-SCOBI	16
2.12.	Black Sea Coupled dynamics and biogeochemical model.....	16
3.	Community models	18
3.1.	Hubbell's neutral model of biodiversity.....	18
4.	Remote sensing	19
4.1.	Regional model of chlorophyll a and coloured detrital matter absorption based on ocean colour satellite data (regional Chl model)	19
4.2.	Regional model of downwelling radiance for the Black Sea (Regional model of downwelling radiance)	20
4.3.	Regional spectral primary production model for the Black Sea (regional spectral PP model)	22
4.4.	Regional inherent optical properties model for the Black Sea (IOPs model).....	23
4.5.	The Particle Size Distribution (PSD) model for the Black Sea (PSD/PSC model)	24
4.6.	Primary production model based on optical properties	25
5.	Habitat models	26
5.1.	Ecological-Niche Factor Analysis and habitat suitability map production	26
5.2.	Process-driven habitat modelling approach	27
5.3.	Habitat suitability based on Generalised Linear Models (GLM) and Generalised Additive Models (GAM).....	28
5.4.	Habitat suitability based on MaxEnt	29
5.5.	NTM (Niche-Trait Model)	29
6.	Food-web models	30
6.1.	OSMOSE model	30
6.2.	SMS	31
6.3.	LeMANS size structured multispecies model.....	32
6.4.	Population-Dynamical Matching Model (PDMM).....	33
6.5.	Threshold-General Additive Models (tGAMs).....	34
6.6.	Qualitative model	34
6.7.	Ecopath with Ecosim and Ecospace	36

1. Hydrodynamic models

1.1. ROMS

ROMS (Regional Ocean Model System) is a free-surface, terrain-following, primitive equations 3D prognostic ocean model widely used by the scientific community for a diverse range of applications (e.g., Haidvogel *et al.*, 2000; Marchesiello *et al.*, 2003; Peliz *et al.*, 2003; Di Lorenzo, 2003; Dinniman *et al.*, 2003; Budgell, 2005; Warner *et al.*, 2005a, b; Wilkin *et al.*, 2005). The algorithms that comprise ROMS computational nonlinear kernel are described in detail in Shchepetkin and McWilliams (2003, 2005), and the tangent linear and adjoint kernels and platforms are described in Moore *et al.* (2004). It simulates the salient features of the large-scale circulation patterns as well as the mesoscale features of the marine ecosystem. It is a split-explicit and free-surface model which considers the Boussinesq and hydrostatic assumptions when solving the primitive equations. In the vertical, the primitive equations are discretized over variable topography using stretched terrain-following coordinates (Song and Haidvogel, 1994). The stretched coordinates allow increased resolution in areas of interest, such as thermocline and bottom boundary layers. In the horizontal, the primitive equations are evaluated using boundary-fitted, orthogonal curvilinear coordinates on a staggered Arakawa C-grid. The general formulation of curvilinear coordinates includes both Cartesian (constant metrics) and spherical (variable metrics) coordinates. Coastal boundaries can also be specified as a finite-discretized grid via land/sea masking. The both vertical and horizontal stencils utilize a centred, second-order finite differences. However, the code is designed to make the implementation of higher order stencils easily. ROMS is forced by detailed atmospheric, hydrologic and oceanic forcing. The rivers runoff data are prescribed as boundary conditions on momentum, salinity, temperature and nitrate. ROMS is coupled to biogeochemical models such as N₂P₂Z₂D₂ and BIOEBUS.

1.1.1. References

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1.2. POM

POM is a 3D hydrodynamic model oftentimes referred as the Princeton Ocean Model (POM), numerical model for ocean circulation used to simulate and predict oceanic currents, temperatures, salinities and other water properties (Blumberg and Mellor, 1987). POM is a sigma coordinate, free surface ocean model with embedded turbulence and wave sub-models, and wet-dry capability. Complete thermodynamics are implemented. POM provides the background physical information for biogeochemical models as BFM, ERSEM, BIMS.

1.2.1. References

Blumberg, A.F., Mellor, G.L., 1983. Diagnostic and prognostic numerical circulation studies of the South Atlantic Bight. *J. Geophys. Res.* 88 (C8), 4579–4592.

For more details and references please refer to:

<http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/index.html>

1.3. NEMO

NEMO is a 3D hydrodynamic modelling framework that produces in space and time variables as velocity field, a linear or non-linear sea surface height, temperature and salinity. In the horizontal direction, the model uses a curvilinear orthogonal grid and in the vertical direction, a full or partial step z-coordinate,

or σ -coordinate, or a mixture of the two. NEMO is able to deal with a wide panel of space and time scales, starting from 1km and a few hours to larger and global space and time scales.

1.3.1. References

For more details and references please refer to: <http://www.nemo-ocean.eu/>

1.4. GETM-GOTM

The 3D General Estuarine Transport Model (GETM, <http://www.getm.eu>) is a three-dimensional free-surface primitive equation model that solves the three-dimensional hydrostatic equation of motion applying the Boussinesq and boundary layer approximations (Stips *et al.*, 2004; Burchard and Bolding, 2002). Horizontal spherical coordinates and vertical, terrain following σ -coordinates are combined to give the required grid spacing and layer distribution. The σ -coordinates are equidistant for shallow water depths, but in deeper water the levels are concentrated at the surface and the bed using a generalised version of the mixed-layer transformation proposed by Burchard and Petersen (1997), in order to better resolve the surface mixed layer and bottom boundary layer. Turbulence is solved vertically by the General Ocean Turbulence Model, GOTM (Umlauf *et al.*, 2006; Umlauf and Burchard, 2005). The variables are arranged on an Arakawa C grid (Arakawa and Lamb, 1977). This is known to be particularly prone to grid scale noise due to spatial averaging of Coriolis terms, but provided the deformation radius is well resolved (~ 30 km), C-grid models yield the most accurate numerical solutions (Adcroft *et al.*, 1999). The free-surface, density and active/passive tracers are located at the centre of the cell, whereas the horizontal velocities (u and v) are located at the west/east and south/north edges of the cell, respectively.

1.4.1. References

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Umlauf, L. and Burchard, H., 2005. Second-order turbulence closure models for geophysical boundary layers. A review of recent work. *Continental Shelf Research*, 25:795–827. U

Umlauf, L., Burchard H. and Bolding K., 2006. General Ocean Turbulence Model. Source code documentation. Technical Report 63pp.

1.5. POLCOMS

POLCOMS is a three-dimensional baroclinic Arakawa B-grid model designed for the study of shelf sea processes and ocean-shelf interaction. It can also be used in estuarine environments. The model solves the momentum and scalar transport equations for oceanographic applications with realistic topography, bathymetry and forcing. The underlying hydrodynamics in POLCOMS are the shallow water equations with the hydrostatic and Boussinesq approximations. This limits model applicability to flows where the vertical acceleration is small and in practice this imposes a minimum horizontal resolution; simulation can be made at resolutions finer than this but at no benefit to the solution. As a rough guide this can be taken as half the maximum water depth. POLCOMS can be coupled to a range of different modelling systems: notably ERSEM, GOTM, BIMS, and the 3rd generation WAve Model (WAM).

1.5.1. References

For more details please refer to: <http://noc.ac.uk/science-technology/research-groups/msm>

1.6. MOHID

MOHID is a three-dimensional water modelling system, developed by MARETEC (Marine and Environmental Technology Research Center) at Instituto Superior Técnico (IST) which belongs to Technical University of Lisbon. The MOHID modelling system allows the adoption of an integrated modelling philosophy, not only of processes (physical and biogeochemical), but also of different scales (allowing the use of nested models) and systems (estuaries and watersheds), due to the adoption of an object oriented programming philosophy. The hydrodynamic model is a free surface, baroclinic model with Boussinesq approximations and considering hydrostatic equilibrium. It uses a finite volume approach with a generic vertical discretization (Martins *et al.*, 2001). The turbulent vertical mixing coefficient is determined using the General Ocean Turbulence Model (GOTM).

1.6.1. References

Martins, F., Leitaó, P., Silva, A., and Neves, R.: 3D modelling in the Sado estuary using a new generic vertical discretization approach, *Oceanologica Acta*, 24, S51-S62, 2001.

2. Biogeochemical models

2.1. N₂P₂Z₂D₂

N₂P₂Z₂D₂ is a biogeochemical model (Fasham *et al.*, 1990) that takes into account ammonium, nitrate, two classes of phytoplankton, two classes of zooplankton and two classes of detritus. The phytoplankton compartments correspond to flagellates (nanophytoplankton) and diatoms (microphytoplankton), and the zooplankton compartments correspond to ciliates (microzooplankton) and copepods (mesozooplankton). The two detrital compartments close the cycling of nitrogen: particulate (PON, large) and dissolved organic nitrogen (DON, small). Dynamics of the multivorous food chains is driven by grazing of mesozooplankton on large phytoplankton and microzooplankton that mainly produces detrital PON, a preferential way for the export of carbon at depth. In contrast, the tight coupling between small phytoplankton growth and microzooplankton grazing, autochthonous nitrogen release and DON remineralisation to NH₄ is assumed to represent the dynamic of the microbial food chain that act as a regeneration loop. The biological variables are expressed in term of nitrogen (μM-N), which is generally assumed to be the main limiting nutrient for phytoplankton growth. The biogeochemical composition of the phytoplankton is considered as constant with time and depth with a C: Chl a ratio of 55:1 mg C (mg Chl a)⁻¹ (Rivkin *et al.*, 1996) and a molar C: N ratio of 106:16 (Redfield *et al.*, 1963).

2.1.1. References

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2.2. ERSEM

The European Regional Seas Ecosystem Model (ERSEM) is a plankton functional type model, developed from a NPZD model, which describes the biogeochemical and plankton cycles. The physical processes affecting the biological constituents are horizontal advection and dispersion, and vertical sedimentation, with the horizontal processes operating on scales of tens of kilometres and the vertical processes on tens of metres (Baretta *et al.*, 1995). ERSEM uses a 'functional' group approach to describe the

ecosystem where the biota is grouped together according to their trophic level (subdivided according to size classes or feeding methods). The three major groups are producers, consumers and decomposers. The phytoplankton community is divided into 4 types: Picophytoplankton (0.2-2 μm), Flagellates (2-20 μm), Dinoflagellates (20-200 μm), Diatoms (20-200 μm , silicate dependent) and the zooplankton community in three groups: Mesozooplankton, Microzooplankton, Heterotrophic nanoflagellates, and a decomposer group (bacteria). The ecosystem is considered to be a series of interacting complex physical, chemical and biological processes, which together exhibit coherent system behaviour. Biological functional growth dynamics include both physiological processes (ingestion, respiration, excretion, egestion, etc.) and population processes (growth, migration and mortality) which are described by fluxes of carbon, nitrogen, phosphate, silicate and oxygen. The mathematics of the model resolves:

- a. Primary producers: carbon production is a function of assimilation minus respiration (basal and activity), excretion, lysis, grazing and sinking;
- b. Bacteria: carbon production is a function of assimilation minus respiration (basal and activity), excretion and grazing;
- c. Zooplankton: carbon production is a function of assimilation minus respiration (basal and activity), excretion, mortality and predation.

Where applicable, production is dependent on light, temperature, and nutrients. Phytoplankton has internal nutrient pools and along with bacteria and zooplankton they have dynamically varying C/N/P ratios. The trophic relations between the functional groups are presented in the form of a food matrix (area/ecosystem dependent) where each element of the particular trophic level with regard to the others. The 3D System coupling of the physics and the biology is done through the following equation:

$$\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x} - V \frac{\partial C}{\partial y} - W \frac{\partial C}{\partial z} + \frac{\partial}{\partial x} \left(A_H \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(A_H \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_H \frac{\partial C}{\partial z} \right) + \sum BF$$

where U, V, W represent the velocity field, A_H the horizontal viscosity coefficient and K_H the vertical eddy mixing coefficient, provided by the POM. $\sum BF$ stands for the total biochemical flux, calculated by ERSEM, for each pelagic group. The dynamics of the lower trophic levels are very much determined by the hydrodynamics (horizontal and vertical transport of nutrients, stratification etc.), which control the resource supply. The higher trophic levels may be both resource-controlled (bottom up) and predation-controlled (top-down).

2.2.1. References

Baretta, J.W., Ebenhoh, W., Ruardij, P., 1995. The European regional seas ecosystem model, a complex marine ecosystem model. *Neth. J. Sea Res.* 33, 233–246.

2.3. BFM

The BFM is a numerical model designed to study stoichiometric relationships in the biogeochemistry of marine ecosystems by describing the dynamics of major marine biogeochemical processes (Vichi *et al.*, 2007). The model extends and advances the original philosophy of ERSEM (European Regional Seas Ecosystem Model, Baretta *et al.*, 1995) in modern coding standards, taking into account pelagic, benthic and sea ice dynamics and the coupling between biogeochemical (e.g. photosynthesis, respiration, grazing) and physical (e.g. the effects of temperature and light) processes in the marine environment. At the moment BFM considers the cycles of nitrogen, phosphorus, silica, carbon, and oxygen in the water dissolved phase, as well as in the plankton, detritus, sea ice and benthic compartments. Plankton dynamics are parameterized by considering a number of plankton functional groups, each representing a class of taxa. BFM plankton functional groups are subdivided in producers (phytoplankton), consumers (zooplankton), and decomposers (bacteria). These broad functional classifications are further partitioned into functional subgroups to create a planktonic food web (e.g. diatoms, picophytoplankton, microzooplankton, etc.). The mathematical relationships between the groups' functionalities are defined following the stoichiometric requirements of basic elements. These requirements are dynamically varying between given maximum and minimum values of element ratios, i.e. BFM is a quota (or stoichiometric) model. The pelagic system (Vichi *et al.*, 2007) resolves in default configuration 54 state variables derived from: 4 phytoplanktoners (diatoms, autotrophic nanoflagellates, picophytoplankton, and other large phytoplankton), 4 zooplanktoners (omnivorous and carnivorous mesozooplankton, microzooplankton and heterotrophic nanoflagellates), bacteria, 9 inorganic constituents for nutrients and gases (phosphate, nitrate, ammonium, silicate, dissolved iron, reduction equivalents, oxygen, carbon dioxide and dissolved inorganic carbon) and 4 organic non-living groups for dissolved and particulate detritus.

2.3.1. References

Baretta, J., Ebenhö, W., Ruardij, P. 1995. The European regional seas ecosystem model, a complex marine ecosystem model. *Netherlands Journal of Sea Research* 33:233-246.

Vichi, M., Pinardi, N., and Masina, S., 2007. A generalized model of pelagic biogeochemistry for the global ocean ecosystem. Part I: theory. *Journal of Marine Systems*, 64, 89-109.

2.4. ECOSMO

ECOSMO (ECOSystem MOdel) is a coupled physical-biogeochemical model (Schrum *et al.*, 2006a, 2006b), with the hydrodynamics based on the HAMSOM (HAMBurg Shelf Ocean Model; Schrum and Backhaus, 1999), a free-surface 3D baroclinic coupled sea-ice model. The prognostic variables of HAMSOM include temperature, salinity, relative sea surface elevation, 3D-transport, vertical exchange coefficients and turbulent air–sea exchange. The model uses a semi-implicit method which allows for a relative large model time step of 20 min and hence for efficient long-term integrations. ECOSMO originally included interactions between 12 state variables (Schrum *et al.*, 2006a), but latterly this has increased to 16 (Wakelin, 2012). The basis of the model is 3 nutrient cycles (nitrogen, phosphorus and silica including three sediment nutrient pools) covering the main macro-nutrients limiting phytoplankton production in shelf seas. The specific nutrients included in the ecosystem block are nitrate, ammonium, phosphate and silicate. Based on availability of these nutrients and light availability, ECOSMO simulates the dynamics of three functional groups of phytoplankton (diatoms, flagellates and cyanobacteria), with the dynamics of each group simulated based on their respective physiological characteristics. The fate of two zooplankton functional groups, microzooplankton and mesozooplankton, are estimated, with the dynamics based on their specific feeding behaviour. Other state variables include nitrite, detritus, dissolved organic matter, biogenic opal, and oxygen. The flow of nutrients and biomass in the model is calculated based on the concept of Redfield stoichiometry (Redfield, 1934; Harris, 1986) using carbon units as a currency. The effects of temperature dependence on plankton growth, respiration and remineralisation rates are not addressed, but temperature dependencies for nitrogen oxidation–reduction reactions are considered. A module for carbon chemistry is available which allows the simulation and projection of ocean acidification in a high CO₂ world. The ecosystem model is based on the following form for the prognostic equation of the state variables:

$$C_t + (\mathbf{v} \cdot \nabla) \mathbf{C} + (w_d) C_z = (\mathbf{A}_v C_z)_z + R_c$$

where C , represents any of the 12 state variables, A_v is the vertical sub-scale diffusion coefficient, $\mathbf{v}=(u,v,w)$ the advective grid scale transport, w_d the additional sinking rate and R_c , the concurrent chemical and biological interactions, which are different for each variable based on specific processes involved defining the dynamics of the components simulated. The mathematics of the model includes/resolves the following major points: the biological interaction terms for the 3 phytoplankton groups are functions of growth, grazing by micro- and mesozooplankton and mortality. Primary productivity of phytoplankton depends on the maximum phytoplankton growth rate limited by light or

nutrients. Micro and mesozooplankton production is a function of available phytoplankton and detritus biomass with mesozooplankton also consuming microzooplankton, and is limited by food availability. Respiration or mortality causes a decrease of biomass due to direct mineralization or converting into detritus. Grazing rates are defined with allowance for selectivity (preference). The budget of organic biomass is closed by the reaction equation of detritus. Detritus increases due to phytoplankton and zooplankton mortality and decreases due to feeding by zooplankton. Remineralization rate of detritus is assumed to be spatially and temporally constant. Uptake rates are estimated from Redfield stoichiometry. Oxidation and reduction rates for nitrification/denitrification are calculated dependent on oxygen and temperature. N_2 production by denitrification is considered as a nitrogen sink. Oxygen is coupled to the nitrogen cycle. Processes included in the model relevant for the oxygen dynamics are production via photosynthesis, nitrification, denitrification, consumption by zooplankton respiration and remineralization of detritus. Hydrogen sulfide produced from denitrification is incorporated as a negative oxygen concentration. Oxygen transfer across the sea surface is taken into account and parameterized by forcing the surface toward the saturated oxygen concentration at a rate dependent on the piston velocity.

2.4.1. References

- Harris, G.P., 1986. *Phytoplankton Ecology. Structure, Function and Fluctuation*. Chapman and Hall, London, New York, p. 384.
- Redfield, A.C., 1934. On the Proportions of Organic Derivations in Sea Water and their Relation to the Composition of Plankton. James Johnston Memorial Volume. Liverpool, pp. 176–192.
- Schrum C., Alekseeva I., St. John M. 2006a. Development of a coupled physical–biological ecosystem model ECOSMO. Part I: Model description and validation for the North Sea. *Journal of Marine Systems*. 61: 79-99
- Schrum, C., Backhaus, J.O., 1999. Sensitivity of atmosphere–ocean heat exchange and heat content in North Sea and Baltic Sea. A comparative assessment. *Tellus* 51, 526–549.
- Schrum C., St. John M., Alekseeva I. 2006b. Development of a coupled physical–biological ecosystem model ECOSMO. Part II: Spatial-seasonal characteristics. *Journal of Marine Systems*. 61: 100-113.
- Wakelin S.L., Daewel U., Schrum C., Holt J., Butenschon M., Artioli Y., Beecham J., Lynam C., Mackinson S., 2012. Eu Project Meece Deliverable Report D3.4 Synthesis report for Climate Simulations Part 3: NE Atlantic/North Sea. 65 pp.

2.5. LIFE: Pelagic Biogeochemical Model

The model is a twelve-component pelagic biogeochemical model comprising producers, consumers, decomposers, organic matter (particulate, dissolved labile and semi-labile), nutrients (nitrate, ammonium, phosphate, silicate acid), biogenic silica and oxygen. Trophic interactions are expressed in terms of material flow of basic elements. Producers, consumers and decomposers are used as broad classes of Living Functional Groups (LFG), as proposed by Baretta and Ruardij (1987). These are

composed by an assemblage of organisms with a distinct role in the biogeochemical processes in marine ecosystems. The model was built around the concept of a Generic Type Model (GTM), a modelling strategy that allows the user to define the number of types inside each LFG. For each LFG this arrangement allows the modelling of n types or species different nutrient dependencies, trophic relations, mix trophic behaviour, rate values, etc., while sharing the same set of primitive equations. As such, each type is specified by a set of parameter values, trophic relations and processes (e.g., mixotrophy). The model is biomass-based and the organisms with the same functional behaviour are expressed by the total biomass of the group. All living organisms and all forms of organic matter have variable stoichiometric elemental ratios. The carbon: nutrient ratios are dynamic, varying between a maximum and minimum value. These limits are defined by the user for each LFG type, and vary freely for organic matter components. Producers have additional state variables for chlorophyll cell content and silica in silica-dependent groups such as diatoms. The model accounts for the biogeochemical cycles of carbon, nitrogen, phosphorus, silica and oxygen. The biogeochemical model was developed inside the MOHID system (www.mohid.com) and all processes and state variable reaction terms are calculated for a control volume, independent from any transport scheme. The control-volume approach consists of dividing the water body into finite segments or control volumes (Chapra, 1997), and solving for each one of them a system of linear equations expressing the interdependence of different properties. When not coupled to a hydrodynamic model, the model becomes a stand-alone non-dimensional application (0D). The model uses an Euler forward scheme (explicit method) as the integration method.

2.5.1. References

- Baretta and Ruardij, 1987. Evaluation of the Ems Estuary ecosystem model. *Continental Shelf Research*, 7 (11–12) (1987), pp. 1471–1476.
- Chapra, 1997. *Surface water-quality modelling*. Civil Engineering Series McGraw-Hill, New York (1997).

2.6. ERGOM-MOM and ERGOM-Fish, the Ecological Regional Ocean Model

The hydrodynamic module of ERGOM is based on the Modular Ocean Model (MOM 3.1) (Pacanowski and Griffies, 2000). A simple surface wave model is integrated into MOM which influences bottom stress and re-suspension. A thermodynamic sea ice model (Winton, 2000) is coupled to the MOM code. The basic properties of the biogeochemical model are described in several works (Fennel, 1995; Fennel and Neuman, 1996; Stigebrandt and Wulff, 1987; Neumann, 2000) and reflect several modifications and improvements made to the model during the years. ERGOM describes the dynamics of nitrogen, oxygen and phosphorus including the inorganic nutrients nitrate, ammonia and phosphate, and particulate

organic matter consisting of phytoplankton (autotrophs), dead organic matter (detritus) and zooplankton (heterotrophs). Autochthonous organic matter is produced from the inorganic nutrients by three functional groups of phytoplankton: diatoms, flagellates and others, and cyanobacteria. Organic material sinks and enters the model sediment as benthic nitrogen and phosphorus. Hydrogen sulfide concentrations are represented by “negative oxygen” equivalents (see also BALTSEM model description). The model is described in details by Neumann (2000). In the model, large cells grow rapidly under nutrient-rich conditions while small cells have a growth advantage under low-nutrient conditions, especially during the summer. Since cyanobacteria are able to fix and utilize nitrogen, the model assumes that phosphate is the only limiting nutrient for this functional group. In addition, owing to their ability to fix nitrogen, cyanobacteria are considered to be a nitrogen source for the system. In the process of sedimentation, a portion of the detritus is mineralized into dissolved ammonium and phosphate. Another portion reaches the sea bottom, where it accumulates as sedimentary detritus and subsequently buried, mineralized or re-suspended in the water column, depending on the velocity of near-bottom currents. Under oxic conditions, some of the mineralized phosphate binds iron oxides and is thus retained in the sediment, becoming liberated when conditions become anoxic. Oxygen development in the model is coupled to biogeochemical processes via stoichiometric ratios, with oxygen levels in turn control processes such as denitrification and nitrification (Neumann, 2010). ERGOM has been further coupled to a fish model with an explicit two-way interaction in an Eulerian model system (Radtke *et al.*, 2012). In the Baltic Sea, the fish stock is dominated by two prey species (sprat and herring) and one predator (cod). The dynamics of the fish model is driven by size (mass-class) dependent predator–prey interactions while the interaction between the biogeochemical and fish model components is established through feeding of prey fish on zooplankton and recycling of fish biomass to nutrients and detritus. The implementation of fish behaviour is done by proposing an algorithm to stimulate fish migration by letting the fish following the food. Also, fish species are guided to their respective spawning areas.

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2.7. BIMS-ECO

The default version of the pelagic food web involves 10 aggregated compartments that comprise the small and large phytoplankton (Ps, Pl), (smaller and larger than 10 μ m), micro- and mesozooplankton (Zs, Zl), opportunistic heterotrophic dinoflagellate *Noctiluca scintillans* (Zn), gelatinous carnivores *Aurelia aurita* (Za) and *Mnemiopsis leidyi* (Zm). Labile pelagic detritus (D), nitrate (N), and ammonium (A) constitute other components of the aggregated ecosystem. Particulate organic material is converted directly to ammonium without explicitly considering the microbial loop mediating the decomposition and remineralisation. This structure and the model formulation have been given by Oguz *et al.* (2001a). The more sophisticated version of the model includes DON, bacteria, oxygen as well as oxidation-reduction reactions near the suboxic-anoxic interface (Oguz *et al.*, 2000, 2001a). An extension of the latter to the case of four phytoplankton groups (diatoms, dinoflagellates, small phytoplankton and coccolithophores) together with the additional phosphorus cycle is described by (Oguz and Merico, 2006). Coccolithope model includes explicit parameterization of calcification process. Earlier process-oriented studies used more simplified ecosystem structures (Oguz *et al.*, 1996; 1999) and Oguz and Salihoglu (2000).

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2.8. BALTSEM, the Baltic Sea Long-Term large-Scale Eutrophication Model

The hydrodynamic module BALTSEM (Gustafsson, 2003) divides the Baltic Sea into thirteen interconnected marine basins each of which is assumed to be horizontally homogeneous but with high vertical resolution. State variables are transported both within and between these basins by the hydrodynamic module, while ecosystem variables are described by the biogeochemical module in terms of basic constituents, such as N (Savchuk and Wulff, 1996; Savchuk, 2002; Savchuk *et al.* 2012). The biogeochemical processes and interactions in the coupled pelagic and benthic systems drive the internal nutrient dynamics within the thirteen basins: nutrient uptake by primary producers, grazing and nutrient excretion by zooplankton, mortality of plankton and sedimentation of particulate nutrients, mineralization in the water column and by the sediments, nitrogen fixation and denitrification, redox alterations of relevant processes. The pelagic system of BALTSEM is represented by three phytoplankton functional groups (diatoms, cyanobacteria, small summers species), zooplankton, detritus (N, P, Si), inorganic nutrients (ammonium, nitrate, phosphate, and silicate) and dissolved oxygen (Savchuk *et al.*, 2012). Heterotrophs are both microzooplankton and mesozooplankton. Differently than other Baltic models (e.g. Eilola *et al.*, 2009; Neumann, 2010), the “splitting” of detritus into individual nutrient variables decouples nutrient cycling from the Redfield ratio and allows, for example, taking into account different stoichiometric composition of phytoplankton and zooplankton. Hydrogen sulfide is presented by “negative oxygen” equivalents: 1 mL of H₂S L⁻¹ = -2 mL O₂ L⁻¹ (Eilola *et al.*, 2011). Three sediment state variables are formulated as pools of bioavailable nitrogen, phosphorus, and silica in the active top layer of sediments. Additionally, a vertically integrated bulk sediment parameterization is implemented in the model. The main features of coupling of transport and transformation processes are comprehensively described in Savchuk *et al.* (2012), where also relevant references of e.g. applied parameterizations of ecosystem functions can be found.

2.8.1. References

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2.9. SPBEM St. Petersburg Eutrophication Model

The St. Petersburg Baltic Eutrophication Model (SPBEM) simulates 3D seasonal ecosystem dynamics in the Baltic and White Seas. In the hydrodynamic module, a sea ice model is coupled to the ocean model based on non-linear primitive equations of motion in the hydrostatic and Boussinesq approximations, and the heat and salt transport equations (Neelov *et al.*, 2003; Myrberg *et al.*, 2010). The hydrodynamic module includes original k-l turbulent closure scheme for vertical mixing and uses Arakawa B spherical grid. The biogeochemical module is based on that of Savchuk (2002) and describes the major biogeochemical fluxes in the pelagic and benthic systems: nutrient uptake by primary producers, grazing and nutrient excretion by zooplankton, mortality of plankton and sedimentation of particulate nutrients, mineralization in the water column and by the sediments, nitrogen fixation and denitrification, redox alterations of relevant processes. SPBEM computes 12 pelagic state variables (diatoms, cyanobacteria, small summer species, zooplankton, nitrogen, phosphorus and silica detritus, ammonium, nitrate, phosphate, silicate and dissolved oxygen) and 3 benthic state variables (nitrogen, phosphorus and silica) in the top active layer of sediments. The model is not coupled to a hydrodynamic model, but the atmospheric and hydrologic components are considered just as given boundary conditions. The core processes of the biogeochemical modules of SPBEM and BALTSEM models are similar and more details on SPBEM can be directly derived by Savchuk (2002).

2.9.1. References

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2.10. BiOEBUS Eastern Boundary Upwelling Systems

BiOEBUS is biogeochemical, nitrogen-based model derived from the $N_2P_2Z_2D_2$ model (Koné *et al.*, 2005) that was successfully used to simulate the first trophic levels of the Benguela ecosystem. The $N_2P_2Z_2D_2$ model takes into account the main planktonic communities and their specificities in the Benguela upwelling ecosystem. Nitrate and ammonium represent the pool of dissolved inorganic N. Phytoplankton and zooplankton are split into small (flagellates and ciliates, respectively) and large (diatoms and copepods, respectively) organisms. Detritus is also separated into small and large particulate compartments. A cumulative layer at the sediment–water interface exists in which sinking particles are stored. Within this cumulative layer the particles cannot be advected; they just accumulate on the sea floor, without further interaction with the overlying waters. In BiOEBUS, there is also a Dissolved Organic Nitrogen (DON) compartment with source terms (phytoplankton exudation, organic excretion of zooplankton, hydrolysis of detritus) and sink terms (ammonification of DON). Nitrite was also included in order to have a more detailed description of the microbial loop: ammonification/nitrification processes under oxic conditions and denitrification/anammox processes under suboxic conditions. These processes are oxygen dependent, so an oxygen equation was also introduced into BiOEBUS with the source term (photosynthesis), the sink terms (zooplankton respiration, bacteria remineralisation) as well as the sea–air O_2 fluxes (Gutknecht *et al.*, 2008; Huret *et al.*, 2005).

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2.11. RCO-SCOBI

RCO-SCOBI is a coupled physical-biogeochemical model of the Baltic Sea consisting of the Swedish Coastal and Ocean Biogeochemical model (SCOBI) and the Rossby Centre Ocean model (RCO) (Eilola *et al.*, 2009; Meier *et al.*, 2011). RCO is a Bryan-Cox-Semtner primitive equation circulation model with a free surface and open boundary conditions. It is coupled to a Hibler-type sea ice model with elastic-viscous-plastic rheology. A simplified wave model is included to calculate the combined effect of wave and current induced shear stress and thus re-suspension of organic matter (Almroth-Rosell *et al.*, 2011). The SCOBI model (Fig. 3) describes the dynamics of nitrate, ammonium, phosphate, phytoplankton, zooplankton, detritus, and oxygen. Phytoplankton consists of three algal groups representing diatoms, flagellates and others, and cyanobacteria (corresponding to large, small and nitrogen fixing cells). The growth rates depend on nutrient concentrations, irradiance, and water temperature. The modelled cyanobacteria also have the ability to fix molecular nitrogen. Organic matter sinks and enters the sediment containing benthic nitrogen and phosphorus. The sediment processes include oxygen dependent nutrient regeneration and denitrification as well as permanent burial of nutrients. For further details of the SCOBI model the reader is referred to Marmefelt *et al.* (1999) and Eilola *et al.* (2009, 2011, 2013).

2.11.1. References

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2.12. Black Sea Coupled dynamics and biogeochemical model

The main part of the Black Sea ecosystem model is a biogeochemical model. The 3D biogeochemical model coupled with the circulation model is based on the one given by Oguz *et al.* (2001). It has one-way coupling with a circulation model through current velocity, temperature, salinity and turbulent diffusivity. The biogeochemical model extends to 200 m depth with 26 z-levels, compressed to the sea surface. It includes 15 state variables. Phytoplankton is represented by two groups, typifying diatoms and flagellates. Zooplankton is also separated into two groups: microzooplankton (nominally <0.2 mm)

and mesozooplankton (0.2– 2 mm). The carnivorous group covers the jelly-fish *Aurelia aurita* and the ctenophore *Mnemiopsis leidyi*. The model food web structure identifies omnivorous dinoflagellate *Noctiluca scintillans* as an additional independent group. It is a consumer feeding of phytoplankton, bacteria, and microzooplankton, as well as particulated organic matter, and is consumed by mesozooplankton. The trophic structure includes also nonphotosynthetic free living bacterioplankton, detritus and dissolved organic nitrogen. Nitrogen cycling is resolved into three inorganic forms: nitrate, nitrite and ammonium. Nitrogen is considered as the only limiting nutrient for phytoplankton growth. All the variables are presented in the model equations in units mmolN/m³. Additional components of the biogeochemical model are dissolved oxygen and hydrogen sulfide. The local temporal variations of all variables are expressed by equations of the general form:

$$\frac{\partial F}{\partial t} + \frac{\partial(uF)}{\partial x} + \frac{\partial(vF)}{\partial y} + \frac{\partial((w + w_s)F)}{\partial z} = K_h \nabla^2 F + \frac{\partial(K_v \frac{\partial F}{\partial z})}{\partial z} + \mathfrak{R}(F)$$

where $\mathfrak{R}(F)$ is the interaction term, which expresses a balance of sources and sinks of each of biological and geochemical variables F ; w_s represents the sinking velocity for diatoms and detrital material and is set to zero for other compartments; (u, v, w) – components of the current velocity, K_h , K_v – horizontal and vertical coefficients of turbulent diffusion. The last parameters are provided by the physical model (the circulation model). The biogeochemical model uses the MHI or POM model output, so its space resolution is equal to the space resolution of the appropriate circulation model (Dorofeev *et al.*, 2011). Fluxes of all biogeochemical variables are set to zero on the sea surface, bottom in the shallow part of the basin and on the lateral boundaries, except river estuaries, where nitrate fluxes are set up proportional to rivers discharges and nitrate concentrations. On the lower liquid boundary in the deep part of the basin concentrations of all parameters are set to zero except ammonium and hydrogen sulfide (sulfide and ammonium pools).

2.12.1. References

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3. Community models

3.1. Hubbell's neutral model of biodiversity

The neutral model of biodiversity developed by Hubbell (1997, 2001) was inspired by MacArthur & Wilson's (1967) theory of island biogeography. In Hubbell's model, all individuals are assumed to have the same prospects for reproduction and death (neutrality). The variability in relative abundances across species is solely due to demographic stochasticity or 'ecological drift'. This model further assumes a separation of spatial scales: demographic processes occur at the local scale of an ecological community, where species may go locally extinct through demographic drift. The local diversity is replenished by immigration at rate m of propagules from a regional species pool. In this large regional pool, drift may also cause species to go extinct, and novel species arise through speciation, such that new species are produced every generation in this regional pool. If $m = 1$, the local community is a random (Poisson) sample of the regional pool. In contrast, if m is close to zero, the local community is virtually isolated from the regional pool. Hubbell's neutral model thus assumes that limited dispersal, rather than niche specialization, is the main explanation for spatial structure across ecological communities. Under this model, the local species abundance distribution is thus defined by only two model parameters, θ and m . A spatially-explicit version of Hubbell's model has also been developed (Chave & Leigh, 2002), in which dispersal from one locale to another is limited by the geographical distance between these sites. In such a model, taxonomic cross-site similarity (i.e. the opposite of β -diversity) declines logarithmically with increasing geographical distance (Hubbell, 2001; Chave & Leigh, 2002). The aim in DEVOTES is to use Hubbell's neutral model framework to assess marine connectivity and biodiversity complementarity. The neutral modelling will be complemented with beta-diversity analysis across the regional seas to infer connectivity in communities occupying the same guild (phytoplankton, zooplankton, macrobenthos). Genetic diversity data will be included to estimate migration among basins at the species level. A connectivity index will be developed showing the need for whole-sea approaches and for interlinked indicators. Specifically, this conceptual model and empirically analysis of cross-sea occurrence data for each community group should permit to propose biodiversity indicators into two approaches: 1) Those communities (or species at genetic level) more vulnerable (i.e. less connected) might be weighted in the biodiversity indices (e.g. AMBI); 2) Those regions with higher beta-diversity (differentiation) should be weighted for conservation priorities.

3.1.1. References

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4. Remote sensing

4.1. Regional model of chlorophyll a and coloured detrital matter absorption based on ocean colour satellite data (regional Chl model)

An algorithm provides a retrieval of chlorophyll a concentration (C_a) and coloured detrital matter absorption (a_{CDM} at 490 nm) in the Black Sea from SeaWiFS-derived normalized water-leaving radiances. A specific approach is needed for the Black Sea, because of the optical complexity of the waters and overlying atmosphere. The algorithm is based on a simple physical model of seawater optical properties formulated in terms of two spectral ratios of normalized water-leaving radiance in SeaWiFS bands 3-5 (Suslin *et al.*, 2008). Parameters of the model are selected empirically with a regional tuning procedure that presumes different water types for shelf and deep water regions of the Black Sea. In situ observations of chlorophyll a concentration and to a lesser extent of coloured detrital matter absorption are used to parameterize and evaluate the algorithm. In comparison to the standard global empirical algorithm for SeaWiFS (OC4), our approach provides accurate estimates of a chlorophyll a concentration within 100-fold range of variability and reveals much more realistic seasonality. Output products (C_a and a_{CDM} at 490 nm) are used as input parameters in several regional models:

- a. the biochemical model (Dorofeev *et al.*, 2011);
- b. the regional models of downwelling radiance (Churilova *et al.*, 2009);
- c. spectral primary production (Churilova *et al.*, 2012);
- d. inherent optical properties (Suslin *et al.*, 2012) and phytoplankton size classes.

4.1.1. References

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4.2. Regional model of downwelling radiance for the Black Sea (Regional model of downwelling radiance)

A. Regional spectral model of downwelling radiance (full version)

The regional approach to the spectral modelling of downwelling irradiance $E_d(z, \lambda)$ is based on the Bedford model (Platt *et al.*, 1991). To take into account the biooptical characteristics of the Black Sea, this model is modified on the basis of the results of parametrization of the absorption of light by the main optically active components in the Black Sea (Churilova *et al.*, 2008). The integral value of PAR incident on the sea surface (SeaWiFS Data) is transformed into the spectral distribution of solar energy according to the data presented in (Shifrin, 1978). The losses caused by the reflection of solar radiation passing through the sea surface are set equal to 6% (Man'kovskii, 1996). The model input parameters: (a) photosynthetically active radiation incident on the sea surface (SeaWiFS Data); (b) sea-surface temperature (SST) (MODIS-Aqua Data); (c) normalized water-leaving radiance at wavelengths of 490, 510, and 555 nm (SeaWiFS Data), used for the evaluation of the surface concentration of chlorophyll a according to the regional algorithm (Suslin *et al.*, 2008). The vertical profile of Chl is retrieved according to (Finenko *et al.*, 2005).

4.2.1. References

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B. Regional simple model of downwelling radiance (SM - simple version)

A simple version (SM) provides a calculation of the spectral diffuse attenuation coefficient of downwelling irradiance ($K_d(\lambda, z)$) in the Black Sea (for depths $z \lesssim 50$ m) using the ocean colour data (Suslin *et al.*, 2011). To simplify regional spectra model of downwelling radiance several assumptions regarding the inherent optical properties (IOPs) of Black Sea waters were used: (a) backscattering was avoided because total backscattering coefficient is much less than the total absorption coefficient; (b) phytoplankton contribution to total light absorption coefficient was avoided because CDM (coloured dissolved organic matter with non-algal particles) was shown to be the main optical component responsible for light attenuation in the Black Sea (Churilova *et al.*, 2008). A standard satellite-derived product of $K_d(490)$ is used as input parameter of SM model, which provides possibility to use the results of SM model in operative mode.

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4.3. Regional spectral primary production model for the Black Sea (regional spectral PP model)

The spectral regional model (Churilova and Suslin, 2012) was based on model of Morel (1991). The regional Black Sea model was developed taking into account regional peculiarities of the biooptical parameters, their difference between seasons, shallow and deep-waters, their depth-dependent variability within photosynthetic zone (Churilova *et al.*, 2008; Churilova and Suslin, 2010). The regional spectral model of primary production includes several regional models:

- a. chlorophyll model, which allows to retrieve surface chlorophyll a concentration (Tchl) and light absorption coefficient of coloured dissolved organic matter in sum with non-algal particles at 490 nm (aCDM(490)) and slope coefficient of aCDM spectral distribution (aCDM(490)) (Suslin *et al.*, 2008);
- b. Tchl profile was retrieved from surface Tchl value following approach (Finenko *et al.*, 2005);
- c. spectral modelling of downwelling irradiance (Churilova *et al.*, 2008).

Input data used in this modelling: 1) photosynthetically available radiation at the sea surface (SeaWiFS data, <http://oceancolor.gsfc.nasa.gov/cgi/level3.pl>); 2) sea surface temperature – SST (MODIS-Aqua data, <http://oceancolor.gsfc.nasa.gov/cgi/level3.pl> and NOAA data, <http://pathfinder.nodc.noaa.gov>); 3) normalized water leaving radiance at 490, 510 and 555 nm - nLw(490), nLw(510), nLw(555) (SeaWiFS data, <http://oceancolor.gsfc.nasa.gov/cgi/level3.pl>).

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4.4. Regional inherent optical properties model for the Black Sea (IOPs model)

A regional algorithm of inherent optical properties (IOPs), such as particle backscattering coefficient at 555 nm ($b_{bp}(555)$), spectral slope of particle backscattering coefficient (n_p), absorption coefficient of sum of coloured dissolved organic matter and non-algal particles (CDM) at 490 nm ($a_{CDM}(490)$), spectral slope of CDM absorption coefficient (S), and chlorophyll a concentration (C_a) derived from SeaWiFS level-2 data, after proper flag/mask and spatial/temporal binning procedures, has been developed (Suslin *et al.*, 2012). The solution was retrieved in each node of the grid by iteration. To improve the stability of the solution, each iteration consisted of three steps (Table 1). At each step, the different components of the IOPs were retrieved using data from different spectral bands. The key step is the first in the Table 1. To calculate the chlorophyll a concentration and CDM absorption coefficient, the regional algorithm developed for the Black Sea (Suslin *et al.*, 2008a, 2008b) is used. A complete set of bi-weekly IOPs maps during SeaWiFS lifetime is available from (Black Sea IOPs maps, 2012). It has been shown that the optical properties of seawater in the Black Sea are typical waters classified as case 2. This means that in general there are no significant correlation values not only between the particle backscattering coefficient and CDM absorption coefficient, but also between the phytoplankton absorption coefficient and CDM absorption coefficient.

Table 1. Description of three sequential steps of one iteration.

Step	Input	Output	Local method
1	$I_s(490)$, $I_s(510)$	$a_{\text{CDM}}(490)$, class of decision	C_a , $\min_{a_{\text{CDM}}(490), C_a, \text{class of decision}} \sum_{\lambda}^{490,510} [I_s(\lambda) - I_m(\lambda)]^2$
2	$R_{\text{RS},s}(490)$, $R_{\text{RS},s}(555)$, $a_{\text{CDM}}(490)$, C_a , class of decision	$b_{\text{bp}}(555)$, n_p	$\min_{b_{\text{bp}}(555), n_p} \sum_{\lambda}^{490,555} [R_{s,\text{RS}}(\lambda) - R_{m,\text{RS}}(\lambda)]^2$
3	$I_s(412)$, $a_{\text{CDM}}(490)$, C_a , $b_{\text{bp}}(555)$, n_p , class of decision	S	$\min_S [I_s(412) - I_m(412)]^2$

Note: the subscripts S and m represent the satellite and model inputs, respectively. $R_{\text{RS},s}$ is a remote sensing reflectance; $I_s(412)$, $I_s(490)$ and $I_s(510)$ are the ratios of $R_{\text{RS},s}(443):R_{\text{RS},s}(412)$, $R_{\text{RS},s}(510):R_{\text{RS},s}(490)$ and $R_{\text{RS},s}(555):R_{\text{RS},s}(510)$, respectively.

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4.5. The Particle Size Distribution (PSD) model for the Black Sea (PSD/PSC model)

The Black Sea Particle Size Distribution (PSD) model was developed using a model proposed by Kostadinov *et al.* (2009), modified taking into account the Black sea peculiarities in spectral slope of particulate backscattering coefficient (Suslin and Churilova, 2012a). The PSDs tend to PSCs for water when we can assume that the backscattering is driven to first order by living cells and their covariates. The model infers phytoplankton size classes from total phytoplankton biomass concentration (in mg C

m-3), that was calculated from chlorophyll a concentration and carbon to chlorophyll ratio (Finenko *et al.*, 2005). Three PSC have been defined, namely, picophytoplankton, nanophytoplankton, and microphytoplankton. Phytoplankton size classes have been estimated from two-weeks IOPs (bbp(555); np; S) maps (Suslin *et al.*, 2012a, b).

4.5.1. References

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4.6. Primary production model based on optical properties

The gross primary production P can be simply modelled from the following equation:

$$P \text{ (mg C m}^{-2} \text{ d}^{-1}) = a * B * Z * I + B$$

where B = phytoplankton biomass (mg chl m⁻³), Z = euphotic depth (metres), I = daily surface irradiance (mol photon m⁻²) and a and B are scaling factors which can be calibrated if real production measurements are available, or taken from the literature (Cole and Cloern, 1987). Phytoplankton biomass can be determined from a range of in-situ sampling techniques and daily irradiance at the surface from an analysis of data from satellites. The depth of the euphotic zone can be determined from observations of light attenuation also from satellites while phytoplankton density from satellites.

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5. Habitat models

5.1. Ecological-Niche Factor Analysis and habitat suitability map production

The ENFA approach, developed by Hirzel *et al.* (2002) computes suitability functions by comparing the species distribution in the eco-geographical variables (EGVs) space, with that of the whole set of cells. For this, independent EGVs describe, quantitatively, some characteristics for each of the cells. The EGV may represent topographical features (e.g., altitude, slope), ecological data (e.g., seagrass cover, nitrate concentration), or human structures, e.g., distance to the nearest coastline, road density. With respect to more standard techniques, a particular advantage in the use of ENFA is that it does not require 'absence data'. The factor analysis method is applied, to transform several correlated variables into the same number of uncorrelated factors. As these factors explain the same amount of the total variance, subsequent analyses may be restricted to the few important factors, e.g., those explaining the largest part of the variance, without losing significant information. The factor analysis may permit the extraction of linear combinations of the original variables, on which the focal species shows most of its Marginality (M) and Specialization (S). M represents the ecological distance between the species optimum and the mean habitat within the reference area (Hirzel *et al.*, 2002). It is defined as the absolute difference between global mean (m_G) and species mean (m_S), divided by 1.96 standard deviations (δ_G) of the global distribution:

$$M = \frac{< m_G - m_S >}{1.92\delta_G}$$

M will lie mostly between zero and one. A large value (close to one) means that the species lives in a very particular habitat, relative to the reference set. The equation is used mainly to explain the principle of the method. The operational definition of Marginality, implemented in the Biomapper 3.2 software, is provided by an equation which is a multivariate extension of the above equation. Similarly, S is defined as the ratio of the standard deviation of the global distribution (δ_G), to that of the focal species (δ_S):

$$S = \frac{\delta_G}{\delta_S}$$

A randomly selected set of cells may be anticipated to have a Specialization of one; any value exceeding unity indicates some form of Specialization. The resulting HS map is defined as a composition of cells, or pixels, whose quantitative values range from 0 to 1 (Hirzel *et al.*, 2006). These values indicate how close the local environment is to the species' optimal conditions; as such, higher values are associated with more suitable areas. The Boyce index from Boyce *et al.* (2002) provides a predicted-to-expected ratio curve, which offers further insights into the model quality: robustness, HS resolution, and deviation from randomness. Such information assists in reclassifying predicted maps, into meaningful HS classes. Thus, the continuous Boyce index is a reliable measure of 'presence-only' based predictions (Hirzel *et al.*, 2006).

5.1.1. References

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5.2. Process-driven habitat modelling approach

The process-driven marine benthic habitat mapping approach, as proposed by Kostylev and Hannah (2007), is based upon ecological theory that relates species life-history traits to the properties of the environment (Huston, 1994; Margalef *et al.*, 1979; Reynolds, 1999; Southwood, 1977), transforming maps of the physical environment into those of benthic habitat types. This approach is based upon the aggregation of sets of environmental selective factors, on two axes. The 'Disturbance' axis reflects the intensity of habitat alteration or destruction, or the durational stability of habitats, including only natural seabed processes responsible for the selection of species' life history traits, on the evolutionary time-scale. The 'Scope for Growth' (SfG) axis, which describes the amount of energy available for growth and reproduction after adjusting the available food supply by environmental stressors that pose a cost for the physiological functioning of organisms. This latter factor could be related also to the metabolic theory of ecology (Brown *et al.*, 2004). Thus, the habitat model constructed according to aforementioned assumptions should reflect the main ecological characteristics of the habitats.

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5.3. Habitat suitability based on Generalised Linear Models (GLM) and Generalised Additive Models (GAM)

Generalized Additive Models (GAMs, Hastie & Tibshirani, 1990) enable the fit of non-linear models for a wide family of statistical distributions. The presence / absence of the species is assumed to follow a binomial error distribution and modelled as:

$$g(m) = a + \sum_i f_i(X_i)$$

where m is the expected probability of occurrence, the linear predictor (on the right hand side) is the sum of the smooth functions (f_i) of the explanatory variables (X_i for $i=1, \dots, p$) and of the intercept a , and the link function that relates the expected probability of occurrence with the linear predictor ($g(m)$) is the logit. Overfitting is prevented by restricting the degrees of smoothness as explained below and by visualizing the response for each variable. GAM model is classified as the semi-parametric extension of Generalized Linear Models (GLMs) (Guisan *et al.*, 2002). GAM is able to realistically model ecological relationships (Austin, 2002) such as asymmetrical niche responses (Oksanen & Minchin, 2002).

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5.4. Habitat suitability based on MaxEnt

Maximum Entropy model (MaxEnt) (Phillips *et al.*, 2006) is a novel machine learning method based on the maximum entropy principle. It is a general-purpose method for characterizing probability distributions from incomplete information (Pearson *et al.*, 2007). This method outperforms many different modelling methods (Elith *et al.*, 2006; Wisz *et al.*, 2008). The MaxEnt model is freely available with MaxEnt software, version 3.3.3k (<http://www.cs.princeton.edu/~schapire/maxent/>).

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5.5. NTM (Niche-Trait Model)

The Niche-Trait Model (NTM) is used to assign habitats and species to positions in an abstract niche space based on the physical characteristics of habitats and the phenotypic traits of species, in such a way that proximity between a species and a habitat in niche space indicates a high preference of this species for that habitat. In other words, the model predicts which species will match which habitat, and explains why. The NTM's mathematical structure follows the theory of Rosberg *et al.* (2010), where the technique was developed in the context of predator-prey interactions. Among the NTM outputs is a ranking of the importance of different direction ("dimensions") in niche space, from which a ranking of the importance of different characteristics (or combinations of characteristics) of species and habitats for determining occupancy of sites can be derived. Variability among species in their most important characteristics according to this ranking can serve as an indicator for functional diversity among species. The models current main applications are benthic habitats and macrobenthos.

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6. Food-web models

6.1. OSMOSE model

OSMOSE (Object-oriented Simulator of Marine ecOSystems Exploitation) is a multispecies and Individual-based model (IBM) which focuses on fish species (Shin and Cury 2001, 2004; Shin *et al.*, 2004). The central hypothesis of the model is that fish predation is opportunistic, based on spatial co-occurrence and size adequacy between a predator and its prey (size-based opportunistic predation). It represents fish individuals grouped into schools, which are characterized by their size, weight, age, taxonomy and geographical location (2D model), and which undergo major processes of fish life cycle (growth, reproduction, recruitment, migration and mortality from predation, natural and starvation) and a fishing mortality distinct for each species. The model takes a wide parameterisation for each fish species and is area specific according to local populations. The species parameterized depend on their local importance related to their biomass, catch and consumption (predator/prey). The model is overall constrained by carrying capacity, with each species governed by its explicit life cycle (standard von Bertalanffy growth, mortality (starvation and fishing) and reproduction equations: see Shin and Cury, 2001), but with interactions through predation modelling involving foraging, min/maximum thresholds for predator/prey size ratios, spatio-temporal co-occurrence and maximum ingestion rates. The model needs basic parameters that are often available for a wide range of species, and which can be found in FishBase. In output, a variety of size-based and species-based ecological indicators can be simulated and converted to in situ data (surveys and catch data) at different levels of aggregation: at the species level (mean size, mean size-at-age, max size, trophic level etc), and at the community level (slope and intercept of size spectrum, Shannon diversity index, etc.). The model can be calibrated to observed biomass, using genetic algorithms. The coupling process used to link OSMOSE to LTL (low trophic level) models (e.g. NPZD, BFM, ERSEM) is the predation process (Travers *et al.*, 2009). The LTL model is used as a prey field for the HTL model (concentration of nitrogen/carbon converted into wet biomass) and the HTL model provides a predation mortality field for the LTL model.

6.1.1. References

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6.2. SMS

SMS is a stochastic multispecies model describing stock dynamics of interacting stocks linked together by predation. It operates on annual or seasonal time steps. The model consists of sub-models of survival, fishing mortality, predation mortality, survey catchability and stock-recruitment (Andersen *et al.*, 1977; Lewy and Nielsen, 2003). SMS uses maximum likelihood to estimate parameters and the total likelihood function consists of four terms related to observations of international catch at age, survey catch per unit effort (cpue), stomach contents observation, and a stock-recruitment (penalty) function. Uncertainties of parameters and biological key parameters (biomass and average fishing mortality) are estimated from the inverse Hessian matrix, or alternatively using the Markov Chain Monte Carlo (MCMC) methodology (e.g. Gilks *et al.*, 1996). The model developed is a mixture of age and size structured models. The catch model has been chosen to be age-structured while the food preference model is size based because preference depends on size rather than age. This also applies to the fishery mortality model as well, but catch data by size classes are generally not available. The mixed age-size structure implies that data by age groups are transformed to sizes using age-length keys. SMS can be used as assessment model, where parameters and the historical stock dynamic are estimated. As forecast model, SMS uses the parameter estimates and terminal stock sizes to forecast stock dynamic in short or long term, given harvest control rules for the individual stocks.

6.2.1. References

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Lewy, P., and Nielsen, A. 2003. Modelling stochastic fish stock dynamics using Markov Chain Monte Carlo. ICES J. Mar. Sci., 60: 743-752.

6.3. LeMANS size structured multispecies model

The length-based multispecies model (LeMANS) (Hall *et al.*, 2006) describes the population dynamics of fish species with defined life-histories, structured in length classes. In the LeMANS model, animals grow towards an asymptotic size following the von Bertalanffy growth model, and reproduce according to a Ricker stock-recruit relationship. Mortality includes three components: (1) non-predation mortality, a U-shaped function of length; (2) predation mortality, which depends on predator-prey size ratios, predator abundance (with a Holling type-II functional response), and a diet matrix (3) fishing mortality (F) depends both on species (some species are fished and others are not) and size (Roche *et al.*, 2011). The model is dependent on life-history parameters and diet information that can be assembled from scientific literature. Estimates of the density-dependent stock recruitment parameter for the Ricker relationship have been derived for Georges Bank and the North Sea following the meta-analytical approach of Hall *et al.* (2006). For the North Sea fish community, the maximum spawning-stock biomass was derived from a combination of stock assessments and trawl-survey data for non-assessed species. For species without stock assessments, biomass estimates can be taken from trawl surveys once adjusted for species-specific catchability. Maturity ogives can be taken from stock assessments or simply set as “knife-edge” functions of length. Fishing mortality in the model depends on both size and species independently:

$$F_{i,l} = F_{full} T_i S(l)$$

where $F_{i,l}$ is fishing mortality of length class l species i , F_{full} is annual fishing mortality rate for a fully recruited fish, T_i is a binary variable indicating whether species i is fished, and $S(l)$ is a selection curve as a function of length. A set of size-selection curves has been used in simulations (Rochet *et al.*, 2011) in an attempt to cover a range of selection curves from trawls to gillnets, i.e. using logistic and normal size selection functions respectively. For a range of commercial species in the North Sea, relative fishing mortality at age was extracted from stock assessments and converted, with the corresponding von Bertalanffy growth parameters, to relative fishing mortality at length. A logistic or normal curve selection pattern was selected based on the best goodness-of-fit to the relative fishing mortality rates.

6.3.1. References

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6.4. Population-Dynamical Matching Model (PDMM)

The PDMM (Rossberg *et al.*, 2008; Fung *et al.*, 2013) aims at reproducing the generic structure of entire marine food webs at species resolution. It overcomes the known problem that most parameterizations of model food webs lead to unfeasible communities (some species go extinct) by constructing model communities through an iterative assembly process, where in each step a few species are added, populations are allowed to respond, and then species that went extinct are removed. Consequently, the PDMM can, in its present form, not reproduce real food webs species-by-species, but only the overall macroecological properties of real food webs. The advantage of using assembled food webs is that empirically unsupported model assumptions to stabilize communities are not required. Stability properties and population-dynamical relaxation times are therefore more likely to correspond with reality than in other cases. An extensive discussion of the PDMM, the underlying model philosophy and model structure, and an analytic theory interpreting the macroecological patterns it generates can be found in a monograph by Rossberg (2013). The current implementation of the PDMM is written in C++. Access to a svn repository of the code can be obtained from Axel Rossberg (Cefas) upon request. The PDMM has been used to predict recovery times for the size structure of marine fish communities (see Fung *et al.*, 2013) and in particular the Large Fish Index (LFI) and the related Large Species Indicator (LSI), the biomass-weighted mean maximum length of fish species (L-max) and the mean maturation length of fish species (L-mat). The PDMM has been parameterized to represent temperate shelf seas communities (Fung *et al.*, 2013).

6.4.1. References

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6.5. Threshold-General Additive Models (tGAMs)

A tGAM model is created statistically in two parts. Firstly, food web dynamics are estimated by separate models for each of the functional groups or species to be modelled (i.e. those groups with time-series data, typically from phytoplankton to fish). This set of separate models is built based on empirical data and emerges from those significant smooth (nonlinear) additive and non-additive (including thresholds) relationships between predictors and the response variable. The model can be formulated to link climatic (temperature) and anthropogenic effects (e.g., fishing, nutrient inputs) on food web interactions where data are available. The non-additive effects can be used to detect regime shifts and quantify the ecological thresholds at which a given predictor changes its relationship with the response variable. The main advantage of such statistical models is the compression of complex dynamics into a simple set of equations with the most parsimonious set of explanatory variables. These properties make this type of model particularly suited to investigate systems where alternative regimes have been described, such as the North Sea (Beaugrand, 2004), the Baltic Sea (Möllmann *et al.*, 2009) and Black Sea (Llope *et al.*, 2011).

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6.6. Qualitative model

“For qualitative system analysis, a food web can be represented by a graph, known as a signed digraph (Levins, 1974), which displays the interactions between variables (here functional groups and fleets) and is constructed using the signs of interactions (+, -, 0), not their magnitude. This means model parameter values are not specified, only their signs. A signed digraph has an equivalent representation in the community matrix (A) where each element a_{ij} represents the direct effect of variable j on variable i . For instance, the direct effect of a predator group on its prey, i.e. removal of biomass through predation, is represented by a negative link, and the direct effect of a prey group on its predators, i.e. biomass creation, gives rise to a positive link. Negative feedback connecting a population to it-self is termed a self-effect. It represents intra-specific competition for space and resources particularly for primary

producers, intra-component predation, and links with the outside system as external recruitment or consumption of species from outside the system (Puccia & Levins, 1985). Dambacher (2001) showed that negative self-effects applied to all system components promoted the stability of the system and the results of associate inverse community matrix. Assuming the model system is at equilibrium, press perturbation analysis corresponds to investigating the expected direction of change (toward a new equilibrium) of each model variable, i.e. its abundance change, following sustained changes in the dynamics (birth or death rates) of one or more model variables. It is carried out by considering the signs of the adjoint of the negative community matrix ($\text{adj}-A$) (Dambacher *et al.*, 2002). In complex systems, a press perturbation may impact a given variable through multiple pathways, a pathway being a suite of direct (e.g. prey and predator) and indirect (e.g. prey of prey) effects that lead from the input (pressed) variable to the response variable. If multiple pathways exist, the resulting responses of a given variable may have opposing signs (increase, +, or decrease, - in abundance). The opposing signs create ambiguity in the predicted responses to change (Dambacher *et al.*, 2002). Weights can be given to the predictions to provide an assessment of the level of ambiguity (Dambacher *et al.*, 2003). For a given response variable, the weight corresponds to the net number of pathways (difference between the number of positive and negative responses) divided by the total number of pathways. Weights range between 0 (complete sign indeterminacy of predictions; sign of overall effect will depend on interaction strength) and 1 (sign completely determined). For investigating model stability, the sign of all feedback loops in the system are inspected. Negative feedback loops maintain a system's equilibrium. Conversely, positive feedbacks magnify changes in variables and drive runaway growth or collapse (refer to Dambacher *et al.*, (2003) for a description of feedback cycles). A model system needs to be stable, at least under certain conditions, for the results of press perturbation analyses to be meaningful. PowerPlay (version 2.0; <http://esapubs.org/Archive/ecol/E083/022/suppl-1.htm>) was used to draw signed digraph (Westfahl *et al.*, 2002) and the "Loop Analysis" facility provided on the "Loop Group" web page (<http://www.ent.orst.edu/loop/>) to perform qualitative and symbolic analysis of the community matrix, including press perturbation analyses corresponding to changes in primary productivity and fishing mortality. For further details on loop analysis, see Puccia and Levins (1985), Dambacher *et al.* (2002) and the web site of the "Loop Group".

6.6.1. References

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6.7. Ecopath with Ecosim and Ecospace

The Ecopath model is based on two main equations. In the first one (Eq.1), the biological production of a functional group is equal to the sum of fishing mortality, predation mortality, net migration, biomass accumulation, and other unexplained mortality.

$$(P/B)_i \cdot B_i = Y_i + \sum_j B_j \cdot (Q/B)_j \cdot DC_{ji} + E_i + BA_i + (P/B)_i \cdot B_i (1 - EE_i) \quad (\text{Eq.1})$$

where (P/B) is the production to biomass ratio for a certain functional group (i), B_i is the biomass of a group (i), Y_i the total fishery catch rate of group (i), (Q/B)_j is the consumption to biomass ratio for each predator (j), DC_{ji} is the proportion of the group (i) in the diet of predator (j), E_i is the net migration rate (emigration – immigration), BA_i is the biomass accumulation rate for the group (i), EE_i is the ecotrophic efficiency, and (1 - EE_i) represents mortality other than predation and fishing. In the second equation (Eq. 2), the consumption of a functional group is equal to the sum of production, respiration and unassimilated food.

$$\text{Consumption} = \text{production} + \text{respiration} + \text{unassimilated food} \quad (\text{Eq.2})$$

The implication of these two equations is that the model is mass-balanced; under this assumption, Ecopath uses and solves a system of linear equations (one for each functional group present in the system) estimating missing parameters. Therefore, the input parameters (B, P/B, Q/B, and DC) are entered first, and then the mass-balance in the model is ensured. To do so, we used the manual mass balanced procedure and we modified the model by adjusting the input parameters of those groups with EE > 1 (Christensen and Walters, 2004).

Ecosim provides temporal simulations using the initial parameters of the Ecopath master equation. It works with a couple of differential equations to estimate biomass fluxes as follows:

$$dB_i/dt = g_i \sum_j Q_{ji} - \sum_j Q_{ij} + I_i - (M_i + F_i + e_i) B_i \quad (\text{Eq.3})$$

where dB_i/dt is the biomass growth rate of group (i) during the interval d_t , g_i is the net growth efficiency (production/consumption ratio), I_i is the immigration rate, M_i and F_i are natural and fishing mortality rates of group (i), e_i is emigration rate (Walters *et al.*, 1997; Christensen and Walters, 2004).

Ecospace is the time- and spatial-dynamic component of Ecopath and considers all the key parameters of Ecosim (Walters *et al.*, 1999). It is based on the same set of differential equations used in Ecosim and performs a complete set of Ecosim calculations for each cell and for each time step. Each cell is linked to the rest of the cells by symmetrical movements (Christensen & Walters, 2004, Christensen *et al.*, 2009). It is graphically represented by a grid map divided into different habitats (e.g., depth, sea floor type) into which the functional groups and fishing fleets are allocated. The distribution of each group depends on habitat preference and is constrained to vertices of adjacent cells. Movement cannot occur diagonally and within a cell species biomass is assumed to be homogenous.

6.7.1. References

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