OCEANOGRAFI Nr 128, 2020

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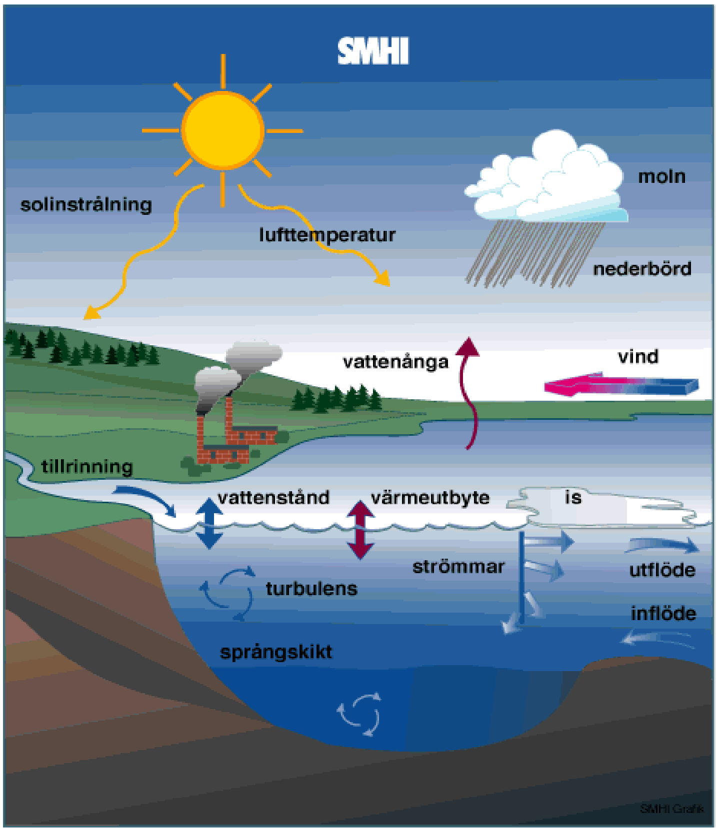

Cover image:
The image visualises physical processes in the coastal zone.

ISSN: 0283-7714

OCEANOGRAFI Nr 128, 2020

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Summary

SMHI develops and maintains a model system for water quality calculations in coastal zone waters around Sweden. It is called the *Swedish Coastal zone Model* (SCM) and has previously been presented in Sahlberg (2009). Since that report was published the model has been further developed and it is now also used in scientific research. This now calls for an updated report.

The SCM is a coupled 1-dimensional physical and biogeochemical model. The model calculates the vertical profiles of all its variables and assumes that they are horizontally homogeneous in the studied area. In order to resolve horizontal variations, a region is divided into several smaller sub-regions, called basins, connected by sounds. Through these sound connections both water and mass of different constituents are exchanged. The basins in SCM are identical to the national water bodies defined in accordance with the Water Framework Directive (WFD). The vertical resolution is half a metre in the uppermost layers, one metre in the 4-70 m interval, and two metres between 70-100 m. Below 100 m the layer thickness increases to 5 m and to 10 m below 250 m.

The physical part of SCM consists of the equation solver *Program for Boundary Layers in the Environment* (PROBE, Svensson (1998)), but also several subroutines which calculates, e.g., insolation, ice-cover, and the exchanges between basins. The exchanges that connect the modelled basins are assumed to be governed by baroclinic and barotropic pressure gradient between the coupled basins.

The biogeochemical model is the *Swedish Coastal Ocean BIogeochemical model* (SCOBI, Marmefelt et al. (2000)). SCOBI is a process-oriented model that includes marine nitrogen, phosphorous and oxygen dynamics, as well as a simple representation of plankton dynamics typical for the Baltic Sea. It calculates 11 variables: zooplankton, three functional phytoplankton groups, detritus, nitrate, ammonium, phosphate, oxygen, benthic nitrogen and benthic phosphorus. SCOBI uses the O_2 variable to also, indirectly, model H_2S. H_2S is represented as a negative oxygen concentration, i.e. the oxygen needed to oxidize a certain accumulated H_2S concentration, which can also be considered as an oxygen debt.

The mixing and advection of the nine pelagic biogeochemical variables are calculated by PROBE, while SCOBI calculates the process rates which decide how matter is exchanged between the 11 biogeochemical variables, and also the vertical transfers between the SCM's grid cells due to the sinking of phytoplankton and detritus, i.e. sedimentation.

SCM needs input data from the atmosphere (weather variables and deposition on nitrogen and phosphorus), from land (land run-off and point sources, e.g. sewage treatment plant and industries) and also from the open ocean.

The model is part of the Swedish water management, but it is also used within research project which results in peer reviewed scientific publications.

Sammanfattning

SMHI utvecklar och underhåller ett modellsystem för beräkningar av vattenkvalitet i Sveriges kustvatten. Modellen kallas Kustzonsmodellen (*Swedish Coastal zone Model*, SCM) och har tidigare presenterats i Sahlberg (2009). Sedan den rapporten publicerades 2009 har modellen utvecklats vidare och den används nu också inom forskning. Detta motiverar nu en uppdaterad rapport.

Kustzonmodellen beräknar både det fysiska och biogeokemiska tillståndet i kustzonen runt Sverige. Modellen simulerar vertikalprofiler för både de fysiska, såväl som de biogeokemiska, variablerna, men bygger på antagandet att de är horisontellt homogena inom ett område. För att beräkna horisontella variationer delas en region upp i flera

mindre underregioner, kallade bassänger, vilka sammankopplas av sund. Bassängerna i kustzonsmodellen är identiska med de nationella vattenförekomster som definieras i enlighet med ramdirektivet för vatten (WFD). Den vertikala upplösningen i modellen är en halv meter i de översta skikten, en meter i intervallet 4-70 m och två meter mellan 70-100 m. Under 100 m ökar skiktens tjocklek till 5 m och till 10 m under 250 m.

Den fysiska delen av SCM består av ekvationslösaren *Program for Boundary Layers in the environment* (PROBE, Svensson (1998)), men också av beräkningsrutiner för till exempel solinstrålning, isbeläggning och utbytet mellan bassängerna. Utbytena som förbinder de modellerade bassängerna beräknas från de baroklina och barotropa tryckgradienterna över sunden.

Den biogeokemiska modellen som används är *Swedish Coastal Ocean BIogeochemical model* (SCOBI, Marmefelt et al. (2000)). SCOBI är en processorienterad modell som inkluderar marin kväve-, fosfor- och syre-dynamik, samt en enkel representation av planktondynamik typisk för Östersjön. Den beräknar 11 variabler: zooplankton, tre fytoplanktongrupper, detritus, nitrat, ammonium, fosfat, syre, bentiskt kväve och bentiskt fosfor. SCOBI använder den modellerade syrekoncentrationen för att också indirekt modellera H_2S. H_2S representeras som en negativ syrekoncentration, d.v.s. det syre som skulle behövas för att oxidera en viss ackumulerad mängd H_2S.

Omlandningen och förflyttningen av de nio pelagiska biogeokemiska variablerna beräknas av PROBE, medan SCOBI beräknar processhastigheterna som bestämmer hur materia utbyts mellan variablerna. Även de vertikala överföringarna mellan SCM beräkningsceller som orsakas av sjunkande fytoplankton och detritus, d.v.s. sedimentation, beräknas av SCOBI.

SCM behöver indata från atmosfären (väder och deposition av kväve och fosfor), från land (landavrinning och punktkällor, t.ex. avloppsreningsverk och industrier) och även från öppet hav.

Modellen är en del av den svenska vattenförvaltningen, men den används också inom forskningsprojekt som resulterar i vetenskapliga publikationer.

Content

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1 INTRODUCTION

SMHI develops and maintains a model system for water quality calculations in coastal zone waters around Sweden. It is called the *Swedish Coastal zone Model*, abbreviated as SCM, and has previously been presented in Sahlberg (2009). Since that report was published the model has been further developed and it has started to also be used in scientific research. This now calls for an updated report.

Previously, the model was used as part of HOME Water where HOME stands for Hydrology, Oceanography and Meteorology for the Environment. Now, the model is still part of the Swedish water management and delivers data to the water web portal (Vattenwebb) hosted by the SMHI, twice each year, but it is also used within research project which results in peer reviewed scientific publications. The SCM is thus used to, e.g., estimate nutrient retention in the Swedish coastal zone (Almroth-Rosell et al., 2016; Edman et al., 2018) and together with satellite data (Kratzer et al., 2019).

SCM is a coupled 1-dimensional physical and biogeochemical model. The model calculates the vertical profiles of all its variables and assumes that they are horizontally homogeneous in the studied area. In order to resolve horizontal variations a region is divided into several smaller sub-regions, called basins, connected by sounds. Through these sound connections both water and mass of different constituents are exchanged. The basins in the Swedish setup of SCM are identical to the national water bodies defined in accordance with the Water Framework Directive (WFD) and divided into five water districts, see fig.1. The geographical constraints of these basins are sometimes changed and they can also be removed or added according to new considerations in management. When this happens, the SCM's geographical setup is updated. However, the approximate number of basins used to model the entire Swedish coast is 650 and they are connected by over 1000 sounds. Each basin is described by its hypsographical curve while the sounds are described by their sill depth, through-flow area and friction. The vertical resolution is half a metre in the uppermost layers, one metre in the 4-70 m interval, and two metres between 70-100 m. Below 100 m the layer thickness increases to 5 m and to 10 m below 250 m.

The biogeochemical model is the *Swedish Coastal Ocean BIogeochemical model (*SCOBI, Marmefelt et al. (2000)). In SCOBI, 11 variables are solved where nine are the pelagic variables: zooplankton, three functional phytoplankton groups, detritus, nitrate, ammonium, phosphate and oxygen. In the benthic layer the model solves for the two variables benthic nitrogen and benthic phosphorus.

2 THE PHYSICAL MODEL

The physical part of SCM consists of the equation solver *Program for Boundary Layers in the Environment* (PROBE), but also several subroutines which calculates, e.g., insolation, ice-cover, and the exchanges between basins. PROBE calculates the transient stratification, mixing and advection in each modelled basin and also the transient concentrations of all state variables. The exchanges that connect the modelled basins are assumed to be governed by baroclinic and barotropic pressure gradient between the coupled basins.

In the following we describe PROBE and the sound exchanges in more detail. In Sahlberg (2009) the ice calculations where described in detail, but they will not be repeated here.

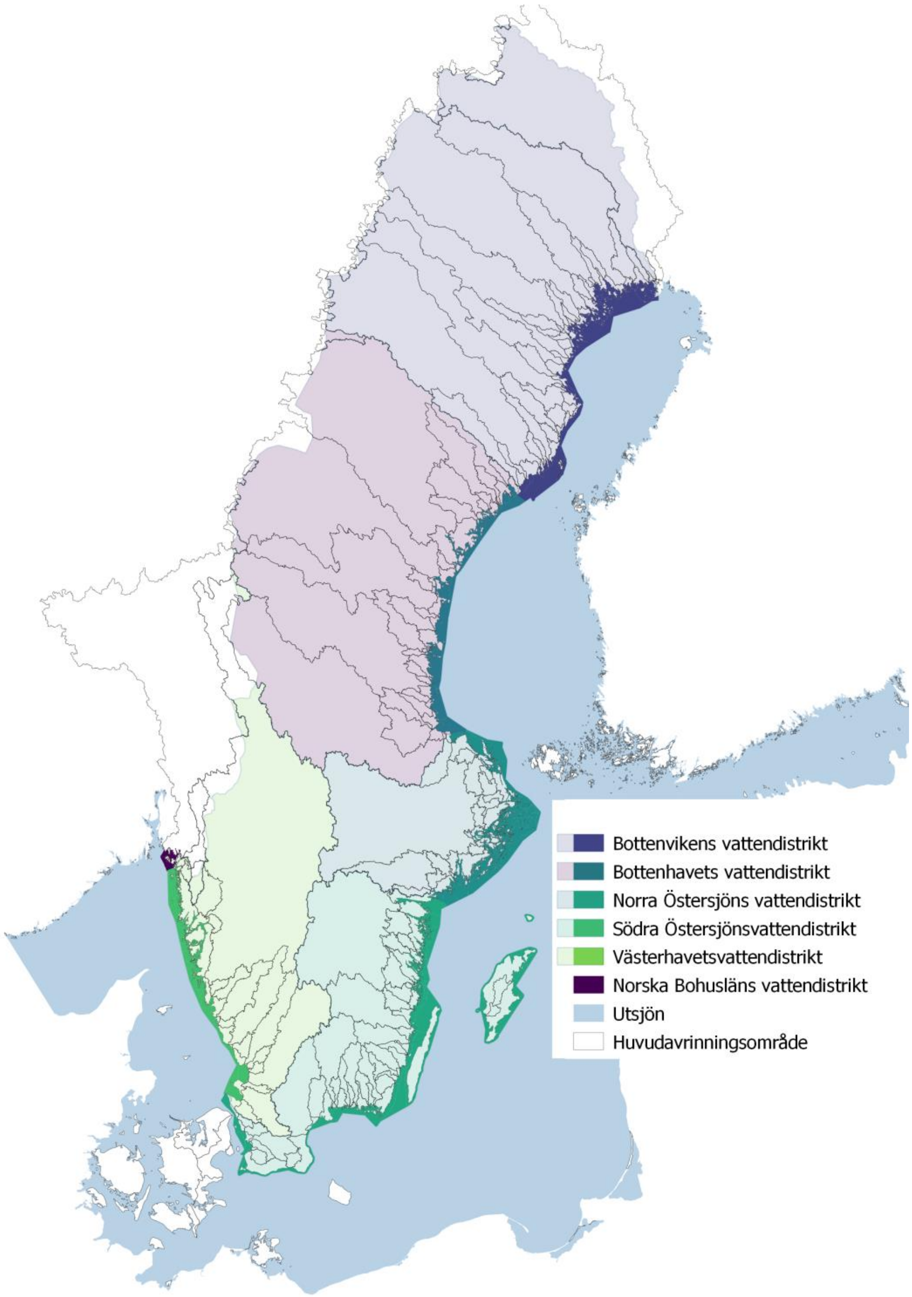

Figure 1. The Swedish Coastal zone Model is set up for the entire Swedish coast, including part of south-eastern Norway to handle runoff from the Glomma river. The Swedish coast is divided into 5 different water districts for administrative purposes.

2.1 The PROBE equation solver

PROBE can be classified as an "equation solver for 1-dimensional transient, or two dimensional steady, boundary layers" (Svensson, 1998). When implemented in the SCM it reproduces the temporal variation of stratification and mixing in each basin. It calculates horizontally averaged concentration profiles of all the state variables. The heat from insolation is distributed in the water column according to a constant attenuation coefficient which is given for each basin in the setup. PROBE embodies a two-equation turbulence model, one equation for the turbulent kinetic energy (k) and one equation for the dissipation of turbulent kinetic energy (ε), and includes a simple parameterisation of deep water mixing.

The general differential equation solved for each dependent, laterally averaged variable, ϕ, in each modelled basin can be written as

$$A\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial z}\left(A\Gamma_\phi\frac{\partial\phi}{\partial z} - Q_z\phi\right) + q_{in}\phi_{in} - q_{out}\phi + \frac{\partial A}{\partial z}J_{\phi bot} \qquad \text{(Eq. 1)}$$

Here t is time, z vertical coordinate, A horizontal area, Γ_ϕ vertical exchange coefficient, S_ϕ source and sink terms per volume, $J_{\phi bot}$ bottom flux per bottom area, Q_z vertical volume flux, and q_{in} and q_{out} horizontal volume fluxes per metre depth to and from the basin through connecting straits. From volume conservations the latter three variables are related through

$$Q_z = \int_{-H_{max}}^{z}(q_{in} - q_{out})dz \qquad \text{(Eq. 2)}$$

where H_{max} is the maximum depth of the basin. The sources and sinks determined by the biogeochemical model are added and subtracted from S_ϕ. Vertical advection and diffusion are excluded for the solution of benthic biogeochemical processes.

The momentum equations read

$$\frac{\partial\rho U}{\partial t} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial z}\left(\frac{\mu_{eff}}{\rho}\frac{\partial\rho U}{\partial z}\right) + f\rho V \qquad \text{(Eq.3)}$$

$$\frac{\partial\rho V}{\partial t} = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial z}\left(\frac{\mu_{eff}}{\rho}\frac{\partial\rho V}{\partial z}\right) - f\rho U \qquad \text{(Eq.4)}$$

where t is time coordinate, x and y horizontal space coordinates, z vertical space coordinate, U and V horizontal velocities, p pressure, f Coriolis parameter, and ρ density. The dynamical effective viscosity, μ_{eff}, is the sum of the turbulent viscosity, μ_T, and the laminar viscosity, μ. Pressure gradients may be treated in several ways, depending on the problem considered.

The surface boundary conditions for the momentum equations are defined as

$$\frac{\mu_{eff}}{\rho}\frac{\partial\rho U}{\partial z} = \tau_x^a \qquad \text{(Eq. 5)}$$

$$\frac{\mu_{eff}}{\rho}\frac{\partial\rho V}{\partial z} = \tau_y^a \qquad \text{(Eq.6)}$$

where $\tau_x^a = \rho^a C_d^a U_i^a W_i^a$ and $\tau_y^a = \rho^a C_d^a V_i^a W_i^a$ are the wind stresses. Wind velocities in x- and y-direction are described by U_i^a and V_i^a and the wind vector is W_i^a. C_d is the drag coefficient and ρ^a is the air density. At the lower boundary the condition of zero velocity is used.

The dynamic eddy viscosity in PROBE is calculated from the turbulent kinetic energy, k, and its dissipation rate, ε, by the Prandtl/Kolmogorov relation :

$$\mu_T = C_\mu\rho\frac{k^2}{\varepsilon} \qquad \text{(Eq.7)}$$

where C_μ is an empirical constant.

The turbulent kinetic energy, k, is given by

$$\frac{\partial k}{\partial t} = \frac{\partial}{\partial z}\left(\frac{\mu_{eff}}{\rho\sigma_k}\frac{\partial k}{\partial z}\right) + P_s + P_b - \varepsilon \quad \text{(Eq.8)}$$

where σ_k is the Prandtl/Schmitt number for k. P_s and P_b are production terms due to shear velocity and buoyancy.

The dissipation rate of turbulent kinetic energy, ε , becomes

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial z}\left(\frac{\mu_{eff}}{\rho\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right) + \frac{\varepsilon}{k}\left(C_{1\varepsilon}P_s + C_{3\varepsilon}P_b - C_{2\varepsilon}\varepsilon\right) \quad \text{(Eq.9)}$$

where σ_ε is the Prandtl/Schmitt number for ε. $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are empirical constants. A full description of the derivation of all turbulence equations and empirical coefficients is found in Rodi (1980) and Svensson (1998).

It should be noted that the SCM implementation of PROBE includes a reduction of the wind estimated for each basin's expanse in the X- and Y- directions, respectively. The reductions are thus set separately for the U- and V- winds. The motivation is to include the energy loss due to the ruggedness of the landscape around a basin. I.e. a narrow width of a basin close to land in, e.g., the X direction should be reflected in a reduction of U wind speed, while wind speeds that act on a basin closer to the open sea would be less reduced. This can be important to differentiate the wind stress within the coastal zone. Especially since the U- and V-wind given to the SCM model are often taken from the coarse grid (relative to the size of some coastal waterbodies) of e.g. atmospheric models or reanalyses data products.

The bottom water eddy diffusivity, ν_z, is commonly expressed as a function of the stability frequency N^2 (Stigebrandt, 1987; Omstedt, 1990) according to

$$\nu_z = \alpha N^{-1} \quad \text{(Eq.10)}$$

where

$$N^2 = -\frac{g}{\rho}\frac{\partial \rho}{\partial z} \ , \quad \text{(Eq.11)}$$

and g is the acceleration of gravity and ρ is the water density. Typical values for α is (1-2) x 10^{-7} (Gargett, 1984; Stigebrandt, 1987; Axell, 1998).

The heat equation in PROBE reads

$$\frac{\partial(\rho c_p T)}{\partial t} + W\frac{\partial(\rho c_p T)}{\partial z} = \frac{\partial}{\partial z}\left(\frac{\mu_{eff}}{\rho\sigma_{eff}}\frac{\partial(\rho c_p T)}{\partial z}\right) + F_{sun}$$

$$F_{sun} = F_s^w(1-\eta)e^{-\beta(D-z)} \quad \text{(Eq. 12)}$$

where T is the water temperature, c_p is the specific heat capacity of water, σ_{eff} is the effective Prandtl number which is the sum of the laminar and turbulent Prandtl numbers, F_{sun} is a source term due to insolation, F_s^w is the part of the total insolation that penetrates the water surface, η is the fraction of F_s^w absorbed in the upper centimetre close to the water surface, β is an extinction coefficient and D the total water depth (note that the z axis starts at the bottom pointing upwards). If the water is ice covered, the short wave radiation that penetrates the water surface is strongly reduced. Equations describing the penetration of short wave radiation through an ice-snow cover are given by Sahlberg (1988)

For the heat equation the surface boundary condition may be formulated as

$$\frac{\mu_{eff}}{\rho\sigma_{eff}}\frac{\partial\rho c_p T}{\partial z} = F_n \qquad \text{(Eq.13)}$$

where F_n is the net heat exchange through the water surface. It consists of the sum of four different heat fluxes

$$F_n = F_h + F_e + F_{nl} + \eta F_s^w \qquad \text{(Eq.14)}$$

where F_h, F_e, F_{nl} are the sensible and latent heat fluxes and net longwave radiation respectively and η is the part of the short wave radiation that is absorbed at the surface. The parameterisation of these fluxes follows from Omstedt and Axell (2003). At the lower boundary a zero flux condition is used, i.e. no sediment heat flux is assumed.

2.2 The water exchanges

In SCM the water exchange between two basins inside the coastal zone or between a coastal zone basin and the outer sea is described in two different ways.

First, the water exchange between two basins within the coastal zone follows from (Stigebrandt, 1990) where the water exchange is controlled by the sum of the barotropic and baroclinic pressure gradients according to

$$Q = \int_0^H B(z)\sqrt{2\alpha(\Delta P_i - \Delta P_s)/\rho_0}\,dz \qquad \text{(Eq.15)}$$

Q is the water flux (m^3s^{-1}), H is the sill depth of the connecting sound (m), B is the width of the sound (m), α is constant set to 0.4, ΔP_i and ΔP_s are the baroclinic and barotropic pressure differences over the sound (Nm^{-2}) and ρ_0 is the water density (kg m^{-3}).

The baroclinic pressure gradient comes from the density difference between the basins calculated from the surface down to the connecting sill depth, see fig. 2.

The water density in basin 1, $R_{1,}$ is smaller than the water density R_2 in basin 2 and thus there is an outflow at the surface from basin 1 to basin 2 and a deeper inflow to basin 1 from basin 2. Net flow to one basin will cause water level rise which generates barotropic currents out of that basin. The route of land discharges through complex archipelagos is therefore calculated by the model.

Inflowing water to one basin seeks there its density level without any entrainment. Heavy surface water in one basin may thus reach the bottom level in the other basin.

Second, the water exchange over the boundary between the coastal zone and the sea is taken from Omstedt and Axell (2003). Normally this boundary is open with a width greater than the internal Rossby radius and the flow is assumed to be in geostrophic balance. The geostrophic balance is formulated as

$$Q = \frac{g\beta\Delta S H^2}{2f} \qquad \text{(Eq.16)}$$

where β is the salinity contraction coefficient equal to 8 *10^{-4}, ΔS is the salinity difference between the deep water and the surface layer and f is the Coriolis parameter. The water exchange is distributed to all depth cells according to their volume. Basically, this exchange causes an adjustment to the open sea at a rate which depends on the strength of the stratification. The sill depth, *H*, is set as an input parameter that can be used to adjust the response time towards open sea forcing.

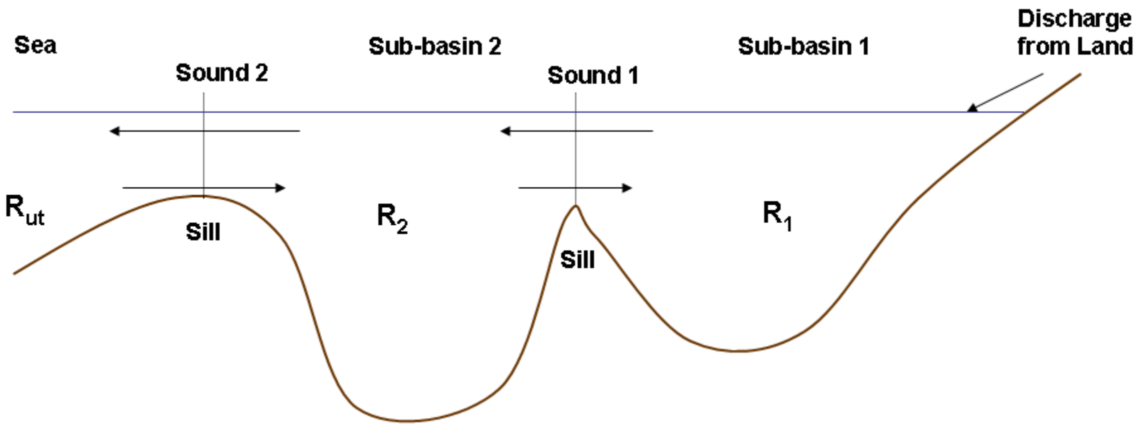

Figure 2. The figure shows the typical water exchange between two basins where basin 1 has a river discharge from land and basin 2 is connected to the sea.

3 THE BIOGEOCHEMICAL SCOBI MODEL

The *Swedish Coastal and Ocean Biogeochemical model*, SCOBI (fig.3) is a process-oriented model that includes marine nitrogen, phosphorous and oxygen dynamics, as well as a simple representation of plankton dynamics typical for the Baltic Sea. This report will give a short description of the main processes and components included in the SCOBI version used by SCM, and their practical implementation. For the full description of the first version of SCOBI see Marmefelt et al. (1999) and for the SCOBI version which forms the basis for the SCOBI in SCM see Eilola et al. (2009).

To describe marine biogeochemistry in a numerical model the main functional parts in the ecosystem (the variables) are identified along with the main processes which should connect those parts. The processes that are used to regulate the marine biogeochemistry in a model are thus links which connect the ecosystem and transfer matter and energy.

SCOBI includes 9 pelagic variables (fig.3); nitrate (NO_3), ammonium (NH_4), phosphate (PO_4), three autotrophic phytoplankton (A1, A_2 and A_3), zooplankton (ZOO), detritus (DET), and oxygen (O_2). SCOBI uses the O_2 variable to also, indirectly, model H_2S. H_2S is represented as a negative oxygen concentration, i.e. the oxygen needed to oxidize a certain accumulated H_2S concentration, which also can be considered as an oxygen debt.

The sediment module (B, fig. 3) in SCOBI includes aggregated process descriptions for nutrient regeneration, denitrification and permanent burial of organic matter. The sediment module contains nutrients in the form of two nutrient variables; benthic nitrogen (NBT) and benthic phosphorus (PBT) which are comparable to available observations of sediment concentrations (Hoefsloot, 2017).

The variables are expressed as concentrations of nitrogen (N), phosphorus (P), carbon (C) or chlorophyll (Chl-a). Carbon is used to represent detritus and zooplankton, while phytoplankton is represented by chlorophyll according to a constant carbon to chlorophyll ratio C:Chl (1:50). To convert units SCOBI uses mole weights and assumes that organic matter consists of C, N and P according to the Redfield ratio (106:16:1, Redfield (1963)).

The mixing and advection of the nine pelagic biogeochemical variables are calculated by PROBE and they are exchanged between basins in the same way as heat or salinity (note that NBT and PBT are not transported through sounds). SCOBI calculates the process rates which decide how matter is exchanged between the 11 biogeochemical variables, and also the vertical transfers between the SCM's grid cells due to the sinking of phytoplankton and detritus, i.e. sedimentation. Included is also the sedimentation of phytoplankton and detritus into the benthic variables.

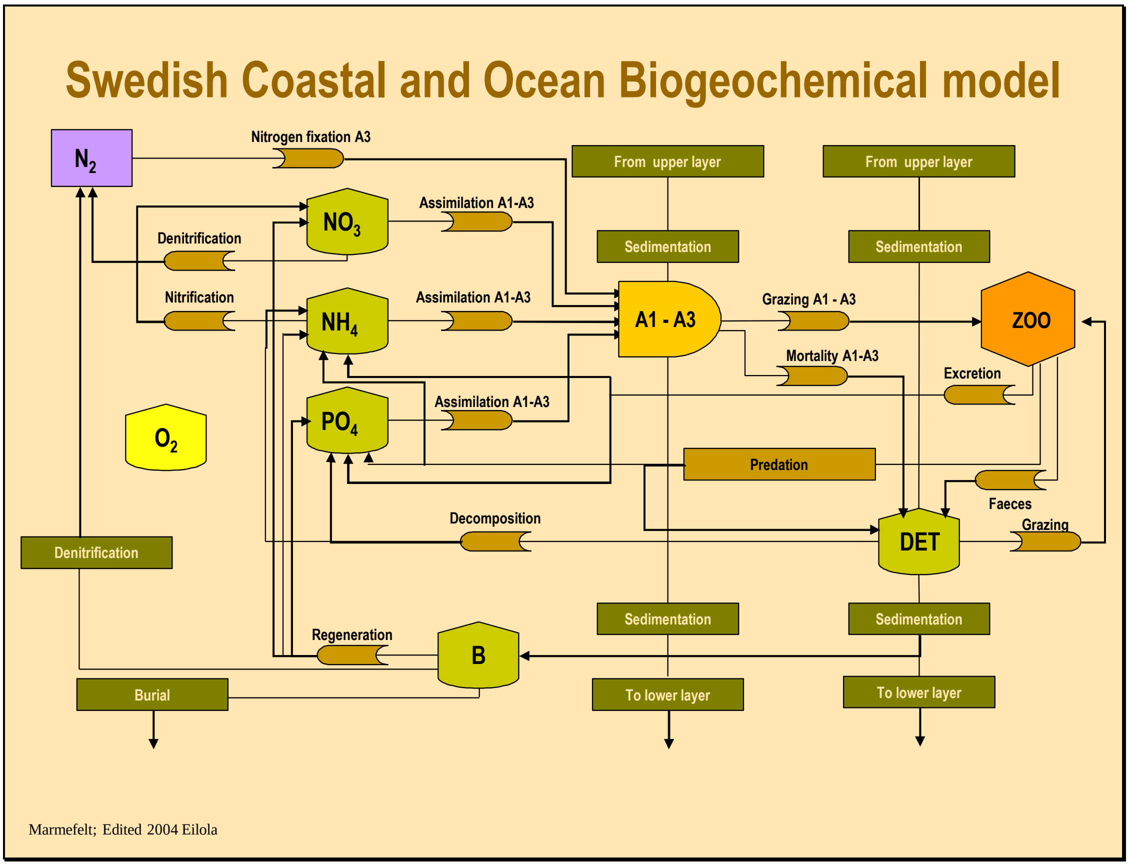

Figure 3. The components of the SCOBI model

The phytoplankton in SCOBI is divided into 3 functional groups with slightly different growth rates, sinking velocities and sensitivities to different kinds of limitations (e.g. nutrients and light). Group A1 is set to represent phytoplankton which bloom early, at the onset of spring, and are often referred to as diatoms. Group A2 grows slower and represents a summer plankton community, e.g. flagellates. Group A3 is set to represent cyanobacteria in water district 1-4, but is used to model the, sometimes toxic, pseudochattonella in water district 1 (the west coast). The cyanobacteria are set to have zero sinking velocity and to be able to grow even if NO_3 and NH_4 are depleted in the model.

In SCOBI, N_2 is assumed to be abundant and never limiting to cyanobacteria growth. It is also assumed to be inert when it is released through denitrification. Thus the amount of N_2 is not calculated, it is just assumed to "be there".

In the following, the biogeochemical processes included in SCOBI will be described and then the processes connecting the nine variables are shown.

3.1 The processes

The 9 pelagic variables in SCOBI can be divided in two groups; the inorganic (O2, NO3, NH4 and PO4) and the organic (A1, A2, A3, ZOO, and DET). The benthic variables PBT and NBT make up a third group.

The processes in SCOBI which transfer matter between the inorganic and organic groups are phytoplankton growth and mineralisation of organic matter. Pelagic mineralization is implemented as decomposition and denitrification of detritus. The processes use different electron acceptors, i.e. oxygen and nitrate, respectively, and the shift from one to the other is regulated by oxygen concentrations. Mineralization also occurs in zooplankton and higher predators as they respire and inorganic matter is thus excreted from these two groups.

However, a large fraction of the mineralization typically takes place in the sediments; especially in shallow basins were organic matter quickly falls into the benthic compartment. Particulate matter that fall into the benthic compartment in SCOBI is added to PBT and NBT according to the Redfield ratio and is subsequently mineralized and released, unless it is buried below the active sediment layer. For each water district a constant fraction is set to be buried deep into the sediment which creates a permanent sink of N and P. The release of nutrients from the sediment is modified by the oxygen concentration in the overlaying water. E.g. if there is not enough oxygen in the overlaying water the ammonia initially formed from mineralization of NBT cannot be nitrified to nitrate and a larger fraction of NBT is released as ammonia. Low oxygen concentration also causes benthic nitrogen to be sequestered, i.e. adsorbed on sediment particles. During the BONUS COCOA project (Carstensen et al., 2019), a formulation of oxygen penetration depth (OPD) was introduced to the model. It enables calculation of how deep into the sediment oxygen can reach, depending on, e.g., sediment porosity.

All mineralization processes that use oxygen in SCOBI are formulated to depend on the amount of substrate and on temperature, while both pelagic and benthic denitrification depends on oxygen, nitrate and organic matter (i.e. detritus or NBT) concentrations.

Phytoplankton growth in SCOBI depends on the concentration of each phytoplankton group and the groups individually set maximum growth rate. The growth rate is then reduced due to limiting factors, i.e. light and the availability of inorganic nutrients. The functional group A3, i.e. cyanobacteria, is set to be able to grow even if NO_3 and NH_4 are depleted in the model and the nitrogen they “assimilate” when they grow without NO_3 or NH_4 replicates the process of nitrogen fixation.

All phytoplankton groups are limited by available light. This constrains their growth during dark winter months and together with the formation of a stable stratification it triggers the spring bloom. However, the underwater light field is not only determined by the amount of light which reaches the water surface, but also the scattering and absorption that attenuate light as it spreads downwards in the water column. The attenuation is calculated as

$$I_z = I_0^{Kd \times z} \qquad \text{(Eq.17)}$$

Where I_0 is the photosynthetically available radiation (PAR) at the surface, z is the distance from the surface, I_z is the PAR at z and Kd denotes the total light attenuation coefficient. Kd is parameterized as

$$Kd=Kd_w+Kd_y+Kd_d+Kd_p \qquad \text{(Eq.18)}$$

where Kd_w, Kd_y, Kd_d, and Kd_p are attenuation due to; water itself, yellow matter, detritus and phytoplankton, respectively. Kd_p depends on the concentration of phytoplankton, hence accounting for the effects of self-shading unto algal growth. Yellow matter mainly consists of humus, i.e. dissolved organic compounds, usually derived from soil and land vegetation. In SCM yellow matter is parameterized from dissolved inorganic nitrogen which in the current SCM version is an inert variable only supplied from river and point sources diluted by sea water.

Between the organic variables matter is transferred according to the processes of grazing, mortality and the production of faecal pellets and particulate waste from higher trophic levels, i.e. predators. Grazing is the only process which increases the zooplankton abundance and zooplankton are assumed to graze both on phytoplankton and on detritus. Mortality, faecal pellets and waste from higher trophic levels are the processes which move phytoplankton, zooplankton and predators to the dead detritus pool, after which they can be mineralized.

There is currently no outtake of fish from the model, and all the nutrients which reach the predator term are returned to the model as inorganic nutrients or detritus.

SCOBI does not include any processes that directly move nitrogen from an oxidized form to NH4, although such processes take place in the marine environment, e.g. ammonification. However, SCOBI does include nitrification which oxidizes NH_4 to NO_3 if there is oxygen available. As a step in the nitrification process nitrite (NO_2) is formed, but since no significant NO_2 concentrations are accumulated, this step, and the NO_2 concentration, has been excluded from the model calculations. If needed, NO_2 can be seen as being embedded in the NO_3 variable.

Oxygen is a part of, or affects, almost all of the processes in SCOBI. It is produced during phytoplankton growth and consumed as zooplankton and predators respire and excrete inorganic constituents. It is also used when dead organic matter is mineralized in both the water column and in sediments. Its' concentration decides if the denitrification is activated in the model and also affects the release of nutrients from the sediment. If there is a lack of oxygen nitrification cannot occur and ammonia accumulates.

To end this section it should be noted that many processes are still not included in SCOBI. However, the most important ones are.

3.2 The sinks and sources

The source terms in Eq.1 for each variable and for each discrete depth layer are described by the equations below. Conversion factors between units are left out for simplicity and clarity. Note that pelagic concentrations are given per unit water volume while the benthic concentrations are given per unit bottom area. Ψ is the ratio between bottom area and water volume. The process descriptions of the SCOBI model are mainly taken from ecological models presented in the literature.

The source terms for the phytoplankton groups are formulated as

$$S_{PHY} = GROWTH_{PHY} + SINKI_{PHY} - SINKO_{PHY} - MORT_{PHY} - GRAZE_{PHY} \qquad \text{(Eq.19)}$$

where *PHY* denotes a phytoplankton group (A1, A2 or A3). *GROWTH* is growth of the phytoplankton population. SINKI is the influx of sinking phytoplankton from the layer above, while *SINKO* is the outflow of sinking phytoplankton to the sediments and to the layer below. Note that A3 does not sink. *MORT* is phytoplankton mortality and *GRAZE* is grazing by zooplankton.

The source term for zooplankton is formulated as

$$S_{ZOO} = GROWTH_{ZOO} - EXCR_{ZOO} - FECAL_{ZOO} - PRED_{ZOO} \qquad \text{(Eq.20)}$$

where *ZOO* denotes zooplankton. *GROWTH* is the sum of grazing from the pools of detritus and phytoplankton. A fraction, *EXCR*, of assimilated food is excreted as inorganic nutrients (ammonium and phosphate) and another fraction, *FECAL,* is lost as faeces to detritus. *PRED* is a closure term representing the predation on zooplankton by higher predators. A fraction (Ω) of *PRED* becomes detritus and the rest is mineralized to inorganic nutrients (ammonium and phosphate).

The source term for detritus is formulated as

$$S_{DET} = SINKI_{DET} + MORT_{PHY} + FECAL_{ZOO} + \Omega \cdot PRED_{ZOO} - GRAZE_{DET} - SINKO_{DET} - DCOMP_{DET} \qquad \text{(Eq.21)}$$

where *DET* denotes detritus. *SINKI* is the influx of sinking detritus from the layer above, while *SINKO* is the outflow of sinking detritus to the sediments and to the layer below. *MORT* is the summarized mortality of the phytoplankton groups. *FECAL* is an input of faecal pellets from zooplankton to the detritus and *GRAZE* is grazing by zooplankton on detritus. Ω ·*PRED* is the fraction of predation that becomes detritus. *DCOMP* is the mineralisation of pelagic detritus to inorganic nutrients (ammonium and phosphate).

The source term for phosphate is formulated as

$$S_{PO_4} = EXCR_{ZOO} + (1-\Omega)\cdot PRED_{ZOO} + DCOMP_{DET} + \Psi \cdot SEDOUT_{PO_4} - UPTAKE_{PO_4} \qquad \text{(Eq.22)}$$

where PO_4 denotes inorganic dissolved phosphate. *EXCR* is excretion from zooplankton, (1 - Ω) · *PRED* is the fraction of predation that becomes phosphate and *DCOMP* is mineralisation of pelagic detritus. *SEDOUT* is flux of phosphate from sediments. The only loss of pelagic phosphate is *UPTAKE* which is the sum of phosphate assimilated during the growth of the phytoplankton groups.

The source term for ammonium is formulated as

$$S_{NH_4} = EXCR_{ZOO} + (1-\Omega)\cdot PRED_{ZOO} + DCOMP_{DET} + \Psi \cdot SEDOUT_{NH_4} - UPTAKE_{NH_4} - NITFIC_{NH_4} \qquad \text{(Eq.23)}$$

where NH_4 denotes inorganic dissolved ammonium. Ammonium is replenished from several sources. *EXCR* is excretion from zooplankton, (1 - Ω) · *PRED* is the fraction of predation that becomes ammonium and *DCOMP* is mineralization of pelagic detritus. *SEDOUT* is flux of ammonium from sediments. Ammonium is lost due to *UPTAKE*, which is the sum of ammonium assimilated during the growth of the phytoplankton groups and *NITFIC* which denotes pelagic oxidation of ammonium to nitrate (nitrification).

The source term for nitrate is formulated as

$$S_{NO_3} = \Psi \cdot SEDOUT_{NO_3} + NITFIC_{NH_4} - UPTAKE_{NO_3} - DENIT_{NO_3} \qquad \text{(Eq.24)}$$

where NO_3 denotes inorganic dissolved nitrate. Nitrogen is replenished by *SEDOUT*, which is flux of nitrate from sediments and *NITFIC*, which denotes pelagic oxidation of ammonium to nitrate (nitrification). Nitrate is lost by *UPTAKE*, the sum of nitrate assimilated during the growth of the phytoplankton groups, and *DENIT*, which is pelagic denitrification of nitrate to N_2.

The source term for oxygen is formulated as

$$S_{O_2} = PROD_{O_2} + DENIT_{NO_3} - DCOMP_{DET} - EXCR_{ZOO} - (1-\Omega)\cdot PRED_{ZOO} - \Psi \cdot RSED_{\Sigma N} - NITFIC_{NH_4} \qquad \text{(Eq.25)}$$

where O_2 denotes dissolved oxygen. The two sources of oxygen is *PROD*, which is the sum of oxygen production due to the photosynthesis, i.e. growth, of the 3 phytoplankton groups, and *DENIT*, which is the reimbursement of oxygen due to pelagic denitrification. Pelagic denitrification occurs to mineralize pelagic detritus if there is a lack of oxygen. Oxygen is consumed in oxidation processes. *DCOMP* is oxygen consumption due to mineralization of pelagic detritus, *EXCR* is oxygen consumption due to zooplankton respiration and (1-Ω) · *PRED* is oxygen consumption due to predator respiration. *RSED* is oxygen consumption due to the oxygen demand by both the decomposition of benthic detritus and benthic nitrification. *NITFIC* is oxygen consumption due to pelagic nitrification.

The source term for benthic phosphorus is formulated as

$$S_{PBT} = SINKI_{PHY} + SINKI_{DET} - SEDOUT_{PO4} - BURIAL_{PBT} \quad \text{(Eq.26)}$$

where *PBT* denotes concentration of labile benthic phosphorus per unit bottom area in the upper "active" sediment layer, usually 2-5 cm. $SINKI_{PHY}$ and $SINKI_{DET}$ are the fluxes to the sediment of sinking phytoplankton and detritus per unit bottom area. *SEDOUT* is a redox dependent flux of phosphate from the sediments. *BURIAL* is permanent burial of phosphorus in layers below the active upper sediment layer.

The source term for benthic nitrogen is formulated as

$$S_{NBT} = SINKI_{PHY} + SINKI_{DET} - SEDOUT_{NO3} - SEDOUT_{NH4} - DENIT_{NBT} - SEQN_{NBT} - BURIAL_{NBT} \quad \text{(Eq.27)}$$

where *NBT* denotes labile benthic nitrogen concentration per unit bottom area in the upper "active" sediment layer. $SINKI_{PHY}$ and $SINKI_{DET}$ are the fluxes to the sediment of sinking phytoplankton and detritus per unit bottom area. $SEDOUT_{NO3}$ and $SEDOUT_{NH4}$ are redox dependent fluxes of nitrate and ammonium from the sediments. *DENIT* is benthic denitrification of nitrate to molecular nitrogen. *SEQN* is redox dependent permanent removal of nitrogen due to adsorption of ammonium to sediment particles. *BURIAL* is permanent burial of nitrogen in layers below the active upper sediment layer.

4 BOUNDARY CONDITIONS

4.1 From the atmosphere

SCM needs meteorological forcing data with 3-hour resolution and the following variables:

- Air temperature (°C)
- U- and V-wind speed (m/s)
- Relative humidity (0-1)
- Cloud cover (0-1)

Until 2009, meteorological data are usually taken from a gridded database developed at the SMHI, the Lars Meuller (LM) database, using meteorological synoptic monitoring station data. Meteorological forcing for 2010 and onwards is taken from the MESAN model, since the LM database was discontinued. The LM database gives geostrophic wind, and the MESAN model gives 10m wind. The LM data is adjusted to 10m in pre-processing and when the MESAN model was implemented to the forcing, the land based grid points were removed since these values were lower due to land surface roughness. This decreased the number of available grid points from 42 to 29. Note that some of these 29 grid points are not used because the forcing for each basin is calculated from the grid point closest to that basin and the extracted set of grid point contain some locations far from the model domain. In pre-processing the wind velocity (speed and direction) is divided in U and V components and adjusted to 10m before 2010. For 2017 onward, data from AROME is used in a similar manner.

Forcing files for atmospheric deposition of nitrogen (NOY and NHX) are usually constructed from MATCH model (Robertson et al., 1999) data (an atmospheric dispersion model that calculates deposition from emissions) and rainfall from the meteorological data.

The forcing has 3-hour resolution and the variables are:

- NOY (mg month^{-1} m^{-2})
- NHX (mg month^{-1} m^{-2})

Phosphorous deposition is not included in the external forcing. Instead it is set in the model code. It is constant over time and the same in all basins. It is set to 0.5 kg km^{-2} month^{-1}, which is equal to 0.5 mg m^{-2} month^{-1}. This value is taken from a report by Areskoug (1993).

For the oxygen equation there is a flux boundary condition at the air-water interface

$$\frac{\mu_{eff}}{\rho}\frac{\partial O_2}{\partial z} = V_{O_2}(O_2 - O_{2sur}(1 + c_{bu})) \qquad \text{(Eq.28)}$$

Here, O_{2sur} is the saturation oxygen concentration at the surface, which depends on temperature and salinity (Weiss, 1970). Stigebrandt (1991) introduced the factor c_{bu} in order to take into account the effects of air bubbles in the surface water. He estimated the value of the "bubble factor" to be c_{bu}=0.025. V_{O_2} is an exchange velocity dependent on wind speed and can be written

$$V_{O_2} = \frac{5.9}{\sqrt{Sc}}(aW + b)\,. \qquad \text{(Eq.29)}$$

Here, Sc is a temperature dependent Schmidt number for oxygen, W is the wind speed and a and b are empirical constants depending on wind speed.

4.2 From land

Land runoff provides water and nutrient input to the coastal zone. Often the S-HYPE model, which is also developed within the SMHI, is used to produce this input. This forcing is the sum of discharges from rivers, land run-off and ground water to the basin. The resolution is daily and the variables are:

- Water flux (m^3/s)
- Total nitrogen (mg/m^3)
- Nitrate (mg/m^3)
- Ammonium (mg/m^3)
- Total phosphorus (mg/m^3)
- Phosphate (mg/m^3)

The nutrient values from S-Hype are given as loads, but the SCM expects concentrations, and hence are the S-HYPE values converted from loads to concentrations by using the water flux. The inorganic nitrogen from S-HYPE is distributed to the NH_4 and NO_3 variables in the forcing by using fractioning constants specific for each water district.

Note that the point sources in S-HYPE are constant over time. However, the nutrient load from land still has transient resolution due to fluctuations of the diffusive sources (i.e. agriculture), correlations between flow and nutrient concentrations and variable retention in lakes and streams.

In SCM the calculated transport data enters the upper 1m layer in the coastal basins. Besides these land discharges there are point sources such as industries and sewage plants with discharges directly into the coastal basins. These point sources are also taken into account in SCM using separate point source files.

The resolution is in the point source files is daily, but usually the point sources have constant values through time since the forcing data is usually taken from the SMED consortium.

The variables in the point source files are:

- Outlet depth (m)
- Water flux (m^3/s)
- Total nitrogen (mg/m^3)
- Ammonium (mg/m^3)
- Nitrate (mg/m^3)
- Total phosphorus (mg/m^3)
- Phosphate (mg/m^3)

Note that the outlet depth set in the files is not used directly in the model. The outlet depth is always set to 5m except when the stratification is considered strong (at least 0.02 increase in density per metre) and Qdepth in the PSR file is deeper than 15m. If both conditions are fulfilled, the outlet depth is set to 15m.

4.3 From the open sea

The conditions in the coastal zone are strongly dependent on the conditions in the open sea outside the coastal zone as the transport over this boundary is large (Eq.15). Normal values of ΔS and mixing depth H along the Swedish coast lead to boundary water transports between $10^3 – 10^5$ m^3/s which are normally much higher than the water transports from land.

The water exchange over the boundary transports heat and salinity for the PROBE model and all nine pelagic variables for the SCOBI model. Thus to get reliable model results in the coastal zone area it is important to know the physical and biochemical conditions in the sea.

Each open sea file should contain daily profiles of the following variables:

- Height over bottom of profile (m)
- Temperature (m^3/s)
- Salinity (g/kg)
- Organic nitrogen ($mmol/m^3$)
- Organic phosphorus ($mmol/m^3$)
- Zooplankton ($mg\ C\ /m^3$)
- Phytoplankton 1 (mg Chl-a$/m^3$)
- Phytoplankton 2 (mg Chl-a $/m^3$)
- Phytoplankton 3 (mg Chl-a $/m^3$)
- Detrital matter ($mg\ C/m^3$)
- Ammonium ($mmol/m^3$)
- Nitrate ($mmol/m^3$)
- Phosphate ($mmol/m^3$)
- Oxygen (ml/L)

The depth-axis starts at the bottom to fit the grid used in SCM.

5 Practical details

SCM can be run on a normal PC or on a computational cluster. The model is rather easy to export to a new coastal zone area as it receives almost all area specific descriptions as input data files. The time step of the PROBE model and the horizontal water fluxes is 10 minutes while the SCOBI variables are calculated once every hour.

The SCM model domain is defined in a setup file which contains information on most aspects of a region, e.g. basins, basin characteristics, basin couplings, sounds and their characteristics, vertical grid and many more. As additional information, each basin needs an initialization file. The initialization file contains the hypsography for the basin and initial concentrations of all needed variables. New versions of these files can be created from model results and existing initial files.

A calculation period should cover at least 20 years, preferably more. The reason for using such a long period is that the nitrogen and phosphorus exchange between the water and the sediments need time to adjust towards a state of equilibrium. If a shorter calculation period is used, it should be kept in mind that the model output might be affected by an imbalance between the models' initial state and its forcing.

The model code and the Swedish setup are kept under version control with subversion. The repository is handled and maintained by the SMHI and versions are archived for each new delivery to the Vattenwebb web portal, i.e. new stable versions are fixed once or twice every year.

The model output is validated regularly as part of the procedure to upload new results to Vattenwebb and as part of scientific peer-reviewed articles or reports (Almroth-Rosell et al., 2016; Wåhlström et al., 2017; Edman et al., 2018; Edman, 2019).

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ISSN:0283-7714