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Development of an Ecological Model System for the Kattegat and the Southern Baltic.

Final Report to the Nordic Councils of Ministers.

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Title (and Subtitle/Titel)

Development of an Ecological Model System for the Kattegat and the Southern Baltic.
(Final Report to the Nordic Council of Ministers).

Abstract/Sammandrag

An integrated ecological model system has been developed that will serve as a first step towards an operational model system for the Skagerrak-Kattegat-Baltic area. The marine biogeochemical model, SCOBI, has been implemented into 3D and has been coupled to the pre-operational hydrological model HBV-N and the atmospheric MATCH model. An improved sediment module is presented.

The SCOBI 3D-model has been coupled to the baroclinic HIROMB model in a 12 nm horizontal grid. The model system has been run for a test period of one year (1997). The validation of the SCOBI 3D-model has been concentrated to the Kattegat-Arkona area. The biogeochemical dynamics of the model for the entire area, however, follows the general pattern of what is known from monitoring. The validation specially points out the sensitivity of the modelled biogeochemical processes in relation to the hydrodynamics.

Key words/sök-, nyckelord

Biogeochemical 3D operational model, integrated ecological model system

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INTRODUCTION

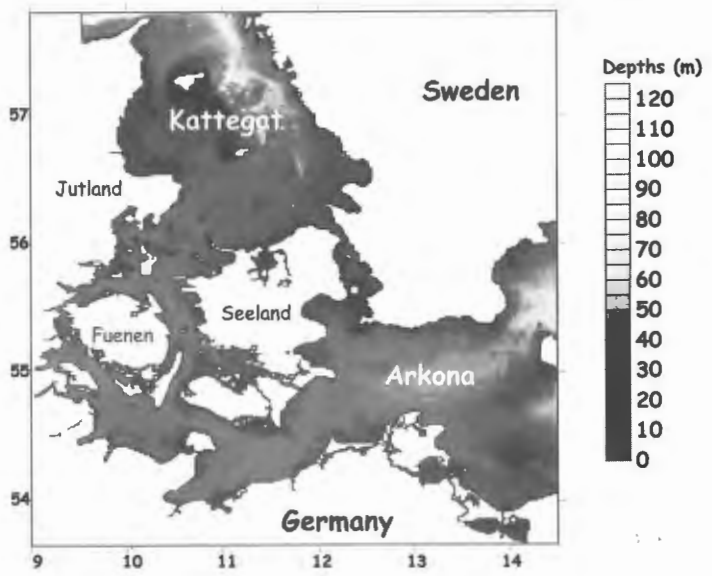


Figure 1 Bathymetric chart of the modelled area

The Kattegat is an area that encounters water quality problems with oxygen deficits in the deep layers and strong eutrophication problems. In particular the Laholm Bay, the Århus Bight and the waters around Funen often affected to oxygen deficits. Fishing capacity losses, especially shell fishing and occasionally harmful algae blooms are other eutrophication effects that has been reported. The area is also exposed to heavy ship- and ferry traffic and fishing.

The Kattegat and southern Baltic are exposed to high riverine nutrient load in the coastal zone. The coastline in the area is fairly open. The Kattegat area itself, can be regarded as a transit area between the Skagerrak and the Baltic Sea with its exposure of intensive water exchange with both the Baltic through the Danish Straits and with the Skagerrak, ANDERSSON & RYDBERG (1993). The external influence from neighbouring water bodies is also an important part of the nutrient cycles, PEDERSEN (1993).

As the coastal zone is exposed both to the open sea and the land, one can expect that also the open sea is highly influenced by the land-based input. In this project we have developed an integrated biogeochemical model system for the Kattegat and the Arkona area. To fully account for the processes taking place between the coastal zone and the open sea we have coupled a biogeochemical model to a 3D numerical model to solve the primitive equations for circulation and mixing. The aim with this project has been to develop an ecological model system for the Kattegat-Arkona area that will serve as a first step towards an operational model system for the Baltic-Kattegat-Skagerrak area, that integrates the marine model system with available atmospheric and hydrological nutrient models.

1 THE SCOBI MODEL

The SCOBI model (**S**wedish **C**oastal and **O**cean **BI**ogeochemical) was first developed as a one-dimensional model with high vertical resolution. It was set up in the Hanoe Bight in the south-western part of the Baltic Sea, MARMEFELT (2000) and MARMEFELT et al. (1999). With the one dimensional approach spatial resolution was taken into account by coupling several model boxes. For transports and mixing, the SCOBI model has to be coupled to a hydrodynamic model. In the one-dimensional model, the SCOBI model is coupled to the hydrodynamical model PROBE. The aim with this project is to go from a one-dimensional model environment into a three-dimensional environment to improve the spatial resolution for the ecological parameters. In order to get there the SCOBI model was coupled to the three-dimensional circulation, turbulence and ice model, HIROMB.

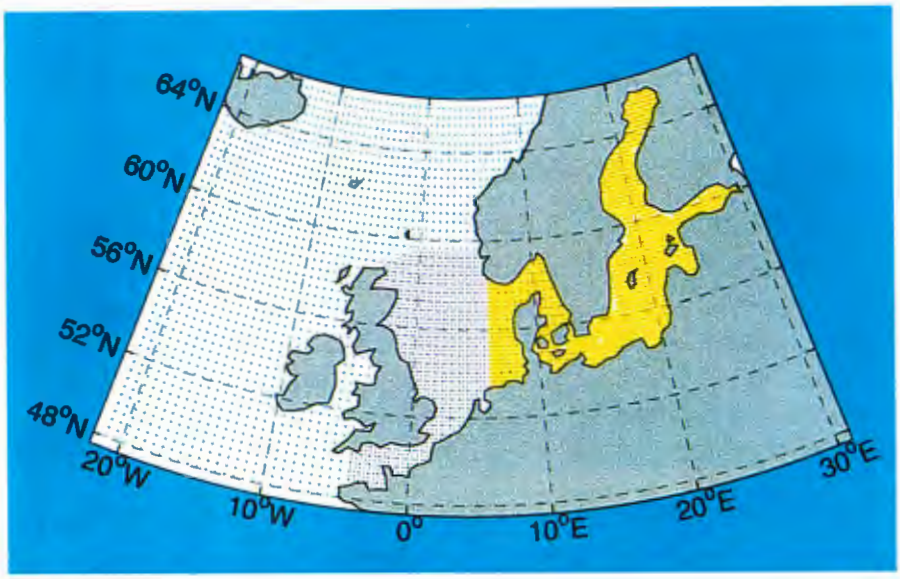


Figure 2 *Modelling area of the HIROMB model. The 12 nm north-eastern Atlantic model is indicated by blue dots, the 3 nm North Sea model area with red dots on white background and the 1 nm Baltic Sea model is indicated by yellow background. The SCOBI model has been implemented in the 1 nm area, but has its open boundary further east at a cross-section between Kristiandsand in Norway and Hanstholm in Denmark.*

The HIROMB (**HI**gh **R**esolution **O**perational **M**odel for the **B**altic Sea) model is a 3D baroclinic model, that is run operationally at the SMHI, FUNKQUIST and KLEINE (2000). The Skagerrak-Kattegat-Baltic area is covered by a 1 nautical mile (nm) grid, which is nested into a 3 nm grid for the same area including the North Sea, Fig. 2. A storm surge model with a coarser horizontal resolution (12 nm) for the north-eastern Atlantic supplies the HIROMB model with water levels at the open boundaries between the Atlantic

and the North Sea. At the same boundary tidal heights and monthly means of salinity and temperature are specified.

The operational HIRLAM model and the HBV model provide the atmospheric and runoff forcing, respectively. Wave-induced mixing in the surface layer together with the Stoke's drift is calculated from the output from an operational wave model (HYPAS).

The SCOBI model has been coupled to the HIROMB model in the 1 nm area. The open boundary towards the North Sea is located at a cross-section between Kristiansand in Norway and Hanstholm in Denmark. At present we have chosen to work with a 12 nm grid in order to develop the coupled model system. With the coarse horizontal resolution, the SCOBI 3D model can be run locally on a UNIX workstation. The SCOBI 3D will, however, be developed into a much higher resolution in the near future.

The vertical resolution of the model is at fixed depths, varying with depth. A finer resolution is set in the surface layers (4 m in the upper 12 m), then gradually turning coarser towards larger depths. The maximum layer depth is 60 m. All together there are 24 vertical layers in the model.

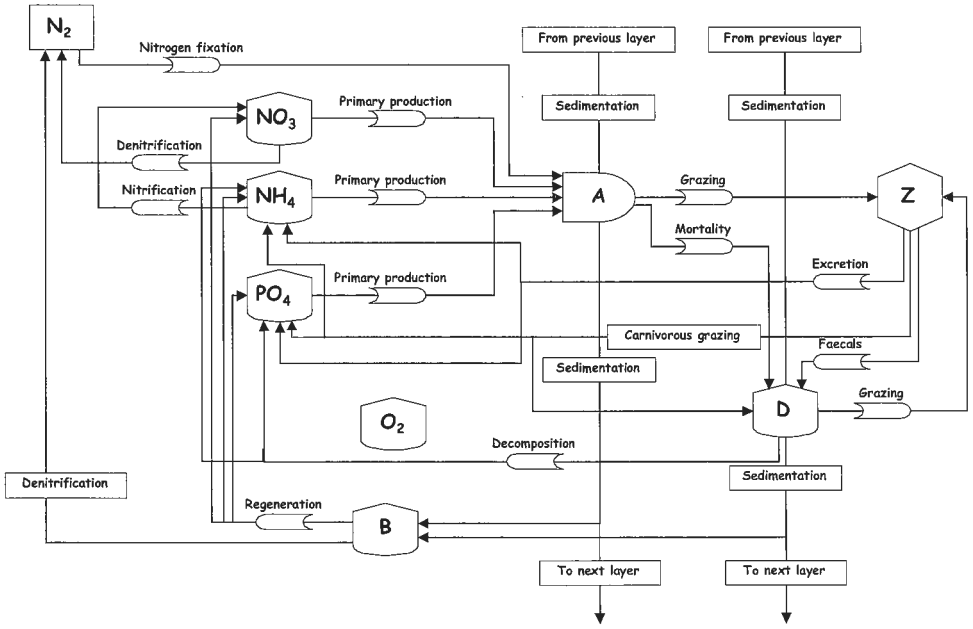


Figure 3 *Schematic illustration of the processes included in the SCOBI model.*

The SCOBI model can be described as a general ecological model, which has been adjusted to the Baltic Sea. Therefore the autotrophs (**A**) in the model include both phytoplankton and cyanobacteria, see Figure 3. During late summer the nitrogen fixation by the cyanobacteria is an important source for nitrogen in the Baltic Proper, KAHRU et al. (1994). Nitrogen fixation has been estimated to approximately 15% of the primary production on an annual basis in the Baltic Proper, see KONONEN (1992). Some years the cyanobacteria bloom is spread as far as to the southern part of Kattegat, but mostly it is captured within the Baltic Proper. Although the primary production in the

Baltic Proper and the Kattegat is regarded as nitrogen limited, GRANELI (1999), during the cyanobacteria bloom the Baltic ecological system turns phosphorous limited. To be able to model these processes phosphate (**PO4**) as well as inorganic nitrogen (**NO3** and **NH4**) has to be included in the model. Silica is not included, as it is not a critical parameter for the primary production, yet. However, declining trends in the ratio between dissolved silica concentration (DSi) and dissolved inorganic nitrogen (DIN) has been observed in the Baltic Sea, RAHM et al. (1996), which may indicate that the spring diatom growth may become silica limited in the future. The fact that the optimal DSi:DIN ratio for diatom growth is approaching 1:1 in the Baltic Sea is a strong argument for including silica in the SCOBI model in the near future.

The limiting nutrient, light and temperature govern the phytoplankton primary production in the model using the Liebig's minimum law. The limiting nutrient is determined by an ordinary Michaelis-Menten expression following DUGDALE (1967), where the phytoplankton preference for ammonia in comparison to nitrate is taken into account. The light limitation of the primary production is following STEELE (1962) and the temperature limitation is a modification of the expression suggested by EPPLEY (1972).

The zooplankton (**Z**) variable represents the zooplankton of the first order. They ingest both phytoplankton (not cyanobacteria) and detritus (**D**), dead organic materia in the model. The closure term of the model system is the carnivorous grazing of the zooplankton. The way the closure term is formulated sets the behaviour of the model. Here the carnivorous grazing is formulated so that the phytoplankton primary production will have an oscillating feature, with an intensive spring bloom and a less pronounced bloom later in the summer, STEELE et al. (1992) and MARMEFELT (2000).

Through faecal production of zooplankton, natural mortality of autotrophs and higher predators, the detritus pool is increased. Detritus is mineralised into ammonia in the water mass. A part of the ammonia is nitrified to nitrate. The excretion of zooplankton ends up as ammonia and phosphate in the model. During anoxic conditions, inorganic nitrogen is lost in the system through pelagic denitrification.

Many of the processes described above are governed by the oxygen concentration. The oxygen concentration ($\mathbf{O_2}$) itself is, however, affected by several processes. In the model oxygen is produced during the photosynthetic primary production and pelagic denitrification. It is consumed through respiration of zooplankton and predators, through decomposition of pelagic and benthic detritus and by the nitrification of ammonia. The oxygen is also exchanged with the atmosphere through the sea surface in a process that is governed by the sea surface temperature and the wind.

Mathematically, the pelagic variables in the model can be described, with tensor notation, as:

$$\frac{\partial \Gamma}{\partial t} + v_i \cdot \frac{\partial \Gamma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(k_i \frac{\partial \Gamma}{\partial x_i} \right) + \Phi_\Gamma ,$$

where the Γ denotes model variables, v_i the velocity components, k_i the kinematic viscosity and Φ_Γ the biogeochemical sinks and sources for the variables. The different sinks and sources are put together in Table 1. The mathematical formulation for the biogeochemical processes in the model is described in appendix A - D.

Table 1 Sinks and sources for the pelagic variables in the SCOBI model

variable (Γ)	**Sinks**	**sources**	**Explanation**
NO3	*ASSIMN*		Phytoplankton assimilation of nitrate
	WDENIT		Pelagic denitrification
		NITR	Nitrification
		REGN	Benthic regeneration
NH4	*ASSIMA*		Phytoplankton assimilation of ammonia
	NITR		Nitrification
		EXCR	Zooplankton excretion
		EXCRPRED	Predator excretion
		DECOMP	Detrital decomposition
		REGA	Benthic regeneration
PO4	*ASSIMP*		Phytoplankton assimilation of phosphate
	NITFIX		Nitrogen fixation
		EXCR	Zooplankton excretion
		EXCRPRED	Predator excretion
		DECOMP	Detrital decomposition
		REGP	Benthic regeneration
A	*SINK*		Phytoplankton sedimentation
	GRAZA		Zooplankton grazing
	MORT		Natural mortality
		ASSIM	Total phytoplankton assimilation
		NITFIX	Nitrogen fixation
Z	*EXCR*		Zooplankton excretion
	PRED		Carnivorous grazing
	FAECAL		Faecali production
		GRAZ	Zooplankton grazing
D	*DECSINK*		Detrital sinking
	DECOMP		Detrital decomposition
	GRAZD		Zooplankton grazing
		MORT	Natural mortality of phytoplankton
		FAECAL	Faecali production
		MORTPRED	Natural mortality of predators
O2	*FOT*		Atmospheric exchange (treated as a source for oxygen when the flow directed from the atmosphere to the sea).
	EXCR		Zooplankton excretion
	EXCRPRED		Predator excretion
	REG		Benthic mineralisation
	NITR		Nitrification
		ASSIM	Phytoplankton assimilation
		WDENIT	Pelagic denitrification

Both detritus and phytoplankton sinks through the water column. In the moment they reach the sea floor, they are mineralised to inorganic benthic nitrogen ($\mathbf{B_N}$) and to inorganic benthic phosphorous ($\mathbf{B_P}$). The mineralisation

process in the model is dependent on temperature and oxygen concentration. In the model $\mathbf{B_N}$ and $\mathbf{B_P}$ are treated as two separate pools.

The fate of the nitrogen pool is dependent on oxygen concentration. During aerobic conditions, the mineralised ammonia is supposed to completely be nitrified to nitrate. Parts of the benthic nitrate (50% as a minimum) are assumed to be denitrified in the anoxic part of the sediment below the redoxcline. The remaining nitrate will be regenerated into the water mass again. The nitrification processes do not take place during anoxic condition, and the regeneration of inorganic nitrogen to the water mass will then be as ammonia.

Also the phosphorous pool is affected by the oxygen concentration. During aerobic conditions parts of the phosphate is adsorbed to particles, the rest is released into the water column. During anaerobic conditions, however, no adsorption takes place. The phosphate is regenerated to the water mass together with some of the previously adsorbed phosphate.

The different sediment pools are mathematically described as:

$$\frac{\partial B_\Gamma}{\partial t} = \Phi_\Gamma,$$

where B_Γ denotes the sediment pool of either nitrogen or phosphorous and Φ_Γ their biogeochemical sinks and sources. Once the nutrients have reached the bottom in the model, they will not be transported, mixed or resuspended in the model. They are solely settled on the sea floor and undergo different biogeochemical processes in the sediments, described in Table 2.

Table 2 Sinks and sources for the benthic variables in the SCOBI model

variable (B_Γ)	Sinks	sources	explanation
B_N	*REG*		Benthic mineralisation
		SINK	Phytoplankton sinking
		DECSINK	Detrital sinking
B_P	*REG*		Benthic mineralisation
		SINK	Phytoplankton sinking
		DECSINK	Detrital sinking

2 SEDIMENT MODULE

To understand the physical and biochemical status of the water body, one has to consider the sediment as a source/sink of nutrients. In the following section some of the important processes in the sediment will be described using Århus Bay as an example, whereas processes such as sedimentation/resuspension and

bedload transport only will be mentioned briefly. A sediment add-on module included in the software package offered at DHI – Water and Environment will also be described in detail, verified by an example from Odense Fjord, Funen.

Due to fertilisation by rivers, coastal upwelling, or the intrusion of deep slope water onto the shelf, about 30 % of the oceanic primary production takes place within the 10 % of the ocean area encompassing shelf and coastal areas. Here, some 25-50 % of the produced organic matter sinks out of the water column onto the sediments, where most of the organic matter is re-mineralised and returned to the water column as inorganic components and only about 10 % of it becomes more permanently buried, JØRGENSEN et al. (1996a).

Even though most of the organic matter is re-mineralised and returned to the water column the sediment does, however, have a large storage capacity for organic matter and nutrients, and the sediments often have an important regulatory and buffering function in the coastal ecosystem, JØRGENSEN et al. (1996a). This is an effect that is enlarged in coastal and shallow water areas, where the sediment in some periods can be the all dominating factor with regard to the water quality.

The main source of organic matter to estuarine and shelf sediments is the deposition of organic matter from the local plankton community in the overlaying water. Consequently, there is a rough correlation between the primary production in the water column, the water depth which detritus sinks while decomposing and the sedimentation of new organic matter to the sediment surface. There are, however, many factors that complicate and delay the coupling of these processes to the benthic metabolism, including temperature, concentrations of dissolved oxygen, degradability, more or less permanent burial in anoxic sediment layers or resuspension and lateral transport of organic matter to deeper or less exposed areas, JØRGENSEN et al. (1996a).

In connection with this it should be mentioned that modelling work on carbon and nutrient cycling in the North Sea, BARRETA et al. (1995), has indicated near bed advection transport of particulate matter to be an important process in creating and maintaining regional differences in the cycling of organic matter and nutrients, by concentrating effective sedimentation in deposition areas.

One of these processes could be bedload transport. Bedload transport in the study area has not been investigated in this project and has until now only been given limited attention in other investigations of marine areas. Therefore, the importance of bedload transport in the Kattegat, the Danish Straits and the Southern Baltic has not been described in any detail. It is, however, believed that bedload transport in the area of interest is less important than the bedload transport in the North Sea. In the North Sea the southern part in particular is effected by bedload transport, which is closely linked to the tidal influence in that area. The tidal range is several meters in the southern part of the North Sea. In the Kattegat and the Southern Baltic the tidal influence is of much less importance, and hence, the effects of bedload transport are also believed to be of less importance.

On the other hand sedimentation and resuspension in the Kattegat and the Southern Baltic can be of great importance. For example, it was observed that organic-rich ephemeral mud blankets in Laholm Bay form on the more sandy sediment surface after sedimentation of the spring bloom of phytoplankton. During successive resuspension cycles these mud blankets were transported out of the bay and into deeper parts of the Kattegat. Similar lateral advection was found to redistribute the deposited organic matter toward the deeper parts of the Kiel Bight in the Western Baltic, JØRGENSEN et al. (1996a). In Århus Bay resuspension is very important in the coupling of processes between water and sediment, by, among other things, transporting nutrients and metals and by stimulating the aerobic degradation. Release of phosphorus was found partly to take place from re-suspended particles, JØRGENSEN (1995). In Århus Bay it was calculated that deposited sediment particles on average were re-suspended into the water column 60 times before permanent burial and during winter storms the resuspension cycle could account for up to 500 g dry matter per m^2 more than 1 1/2 m above the sediment surface in one day. This equals half the yearly net-deposition, JØRGENSEN (1995).

All in all sedimentation/resuspension is of varying importance in the Kattegat and the Southern Baltic but it is not easily assessed in models as resuspension events are closely linked to wind, waves and current and also the size of the particles are very important.

As mentioned at the beginning of this section, the fraction of the primary production in coastal waters deposited on the sediment is normally within the range of 25-50 % of the primary productivity. With a productivity of 250-300 g C/m^2/year in eutrophic coastal waters such as the Kattegat the mean carbon flux to the sediment should be in the range of 75-150 g C/ m^2/year. The annual deposited fraction in the 10-30 m deep Baltic and Kattegat waters was: 26 % in the Southern Kattegat, 32-45 % in Århus Bay and about 30 % in the Kiel Bight, JØRGENSEN et al. (1996a).

Aerobic micro-organisms and animals on the sediment surface primarily mineralise the organic matter, which settles on the sediment surface. The oxic zone of the sediment is, however, restricted to the top few millimetres of the sediment. The degradation and the oxidation of the organic matter below this thin oxic layer is mostly carried out by micro-organisms. Some of these organisms hydrolyse and ferment the macro-molecules to small organic compounds while others use other oxidants than dissolved oxygen. Normally, the most important processes are: 1) the aerobic respiration in the top few mm of the sediment and 2) nitrate respiration (denitrification) in the following mm-cm. Hereafter, other processes such as manganese (Mn) reduction, iron (Fe) reduction, sulphate reduction and finally fermentation take over, JØRGENSEN et al. (1996a).

The iron (Fe) cycle in particular is of great importance as Fe(III) minerals bind inorganic phosphorus (PO4) and thus regulate the release of PO4 from the sediment. When Fe(III) is reduced to Fe(II) phosphorus is released in the pore water of the sediment and consequently PO4 is released to the water column. This process is accelerated when anoxic conditions (< 3 mg O_2/l) occurs or when iron is gradually reduced and reacts with sulphide during summer. In

Århus Bay two occurrences of phosphorus in the water column could be explained by an increased oxidation of organic matter just after spring bloom and during late summer, when degradation of organic matter and denitrification reduced the thickness of the oxic layer and the layer where nitrate was present, JØRGENSEN et al. (1996b). In the study of Århus Bay 32 % of the deposited organic phosphorus was buried into deeper sediment layers. This should be compared to 21 % buried deposited organic carbon and 15 % buried organic nitrogen, JØRGENSEN et al. (1996b).

While 15 % of the deposited organic nitrogen was buried into the sediment the rest was degraded and converted into dissolved organic nitrogen, urea (urea is excreted as a nitrogen waste product by benthic fauna and is also produced by several anaerobic bacteria) and inorganic nitrogen, such as ammonium/ammonia and nitrate. Nitrogen was released from the sediment to the water at relatively constant rates, mostly in the form of urea and ammonium. Urea dominated in the spring period when the sediment was rather oxidised and the concentration of urea in the overlaying layer was low. During periods of anaerobic conditions in late summer the urea was further degraded into ammonium, which was then released, JØRGENSEN et al. (1996b). The overall urea flux appears to be of the same magnitude as the ammonium flux in several coastal sediments, JØRGENSEN et al. (1996a). In Århus Bay the sediment-water flux of nitrate was less important compared to ammonium and urea but especially in the winter period the flux was of the same magnitude as the ammonium and urea fluxes, whereas the flux was negative (from the water to the sediment) in some periods of the summer, JØRGENSEN et al. (1996b).

Some 50-75 % of the produced ammonium was nitrified to nitrate in different shelf sediments of the North Sea, the Kattegat and the Baltic Sea. However, nitrification may be strongly impeded by anoxic conditions with the result that ammonium is released into the water column. Since a large part of the denitrification is dependent on nitrate produced by nitrification, denitrification is also impeded and thereby less nitrogen is removed from the ecosystem. This positive feedback mechanism thus tends to enhance the adverse effects of eutrophication, JØRGENSEN et al. (1996a).

The seasonal variation of nitrate flux from the sediment is regulated by several factors including nitrification, denitrification, and nitrate concentration in the overlaying water, and temperature, JØRGENSEN et al. (1996b).

To summarise the importance of the sediment the case study of Århus Bay will be highlighted, assuming the Århus Bay to some degree represents the Southern part of Kattegat. During one year about 70 % of the nitrogen assimilated in the algae was re-mineralised in the water column. The rest was deposited on the sediment where 85 % was released again as inorganic nutrients and dissolved organic carbon. About 10 % of the deposited nitrogen were lost during denitrification to N_2. This amount equalled half the total amount of direct land based nitrogen load and, thus, the denitrification is significant to the water quality in Århus Bay, JØRGENSEN (1995).

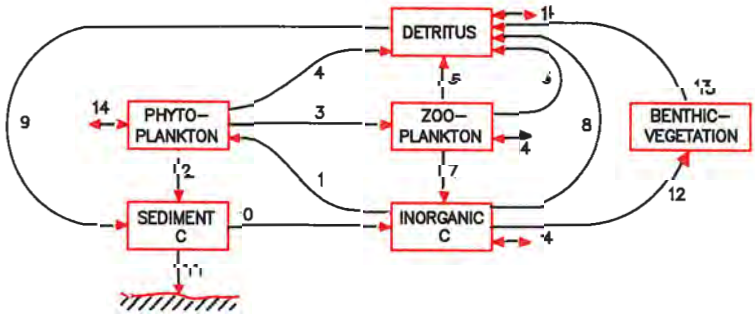
The release of urea and inorganic nitrogen from the sediment was calculated to equal 29 % of the nitrogen, which was required to ensure the measured

primary production. Sources from land immediately surrounding Århus Bay and from the atmosphere contributed with 16-21 % of the primary production, the atmospheric contribution being one third of the terrestrial source, JØRGENSEN (1995). This emphasises the importance of the sediment processes as source/sink in coastal ecosystems.

DHI – Water and Environment has in other projects been involved in modelling the area of interest utilising the software package offered at DHI, MIKE 3 (the DYNOCS project, the BASYS project and at present DHI – Water and Environment is involved in the 'Farvandsmodel' project, which is financed by the Danish EPA and which is used directly in the overall monitoring of the Danish waters).

In connection with the ongoing development of new and better modelling tools, DHI has developed and implemented a sediment module in the standard eutrophication module, which is a part of the MIKE 3 software package. The sediment module has been developed utilising some of the overall findings in the ERSEM model, BARETTA et al. (1995). Within the frame of this project from the Nordic Council of Ministers it has not yet been possible to incorporate the sediment module in the SCOBI model. Instead, the sediment module has been tested as a part of the eutrophication model developed at DHI. The test has been performed on the Odense Fjord system. A broad range of monitoring data exists from this area and it is well known that the sediment has a pronounced effect on the water quality dynamics. The Odense Fjord case therefore gives a good opportunity for calibration and verification of the sediment module.

The standard MIKE 3 eutrophication module (MIKE 3 EU) describes the general eutrophication aspects in the pelagic system, like the nutrient dynamics and growth of phytoplankton with an additional option of including benthic vegetation; macroalgae (mainly Ulva sp.) and rooted vegetation (Zostera marina & Ruppia), DHI (1998b), BACH (1992). The model complex integrates the hydrodynamics (MIKE 3 HD), DHI (1998a), with advection/dispersion (MIKE 3 AD), VESTED et al. (1992).



1. production, phytoplankton
2. sedimentation, phytoplankton
3. grazing
4. extinction, phytoplankton
5. excretion, zooplankton
6. extinction, zooplankton
7. respiration, zooplankton
8. mineralisation of suspended detritus
9. sedimentation of detritus
10. mineralisation of detritus
11. accumulation in sediment
12. production, benthic vegetation
13. extinction, benthic vegetation
14. exchange with surrounding waters

Figure 4 *Processes and state variables in the eutrophication model (MIKE 3 EU) exemplified by the carbon cycle.*

In Figure 4 the state variables and processes for Carbon (C), nitrogen (N) and phosphorus (P) included in the MIKE 3 EU module are presented for the

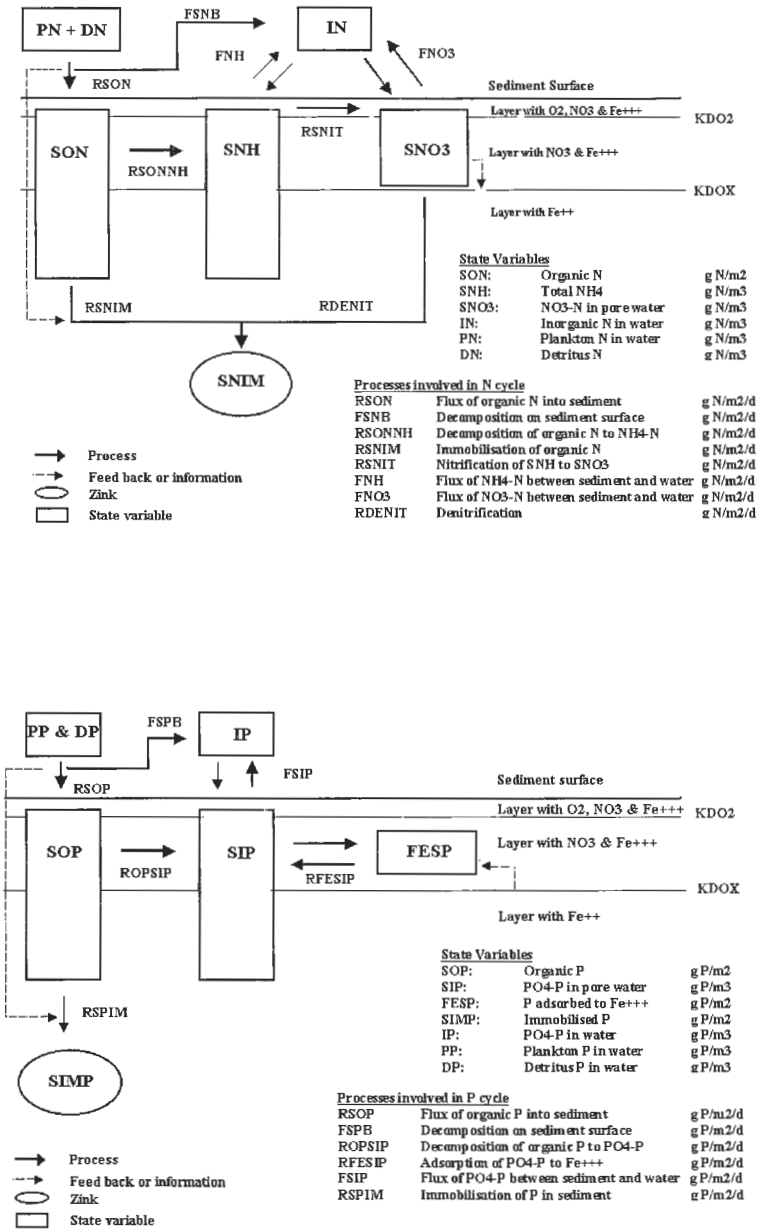


Figure 5 *Diagram of state variables and processes in the sediment N model (top figure) and the sediment P model (bottom figure).*

pelagic system, excluding the enlarged benthic vegetation.

The state variables in the standard module include:

- Phytoplankton carbon, nitrogen & phosphorus
- Chlorophyll-a
- Zooplankton carbon

- Detritus carbon, nitrogen & phosphorus
- Inorganic nitrogen & phosphorus
- Dissolved oxygen

The most important elements in the model are on one hand the growth of phytoplankton, depending on solar radiation, temperature and internal pools of nitrogen and phosphorus in the algae. On the other hand the concentration of phytoplankton is reduced due to sedimentation, grazing and death. Moreover, the decomposition/conversion of organic and inorganic nutrients (carbon, nitrogen & phosphorus) is included in the model.

The sediment module is implemented in the MIKE 3 EU module, thereby making it possible to simulate time-varying nutrient sediment-water fluxes depending upon the location. The nitrogen cycle and the phosphorus cycle are presented in Fig. 4.

As can be seen in Figure 5, the sediment module includes the following state variables:

- Organic nitrogen & phosphorus
- Inorganic nitrogen (ammonium and nitrate) & phosphorus in the pore water
- Phosphorus chemosorbed to oxidised iron and manganese
- Immobilised or buried nitrogen & phosphorus

For a more thorough description of the sediment module please refer to Appendix E - G.

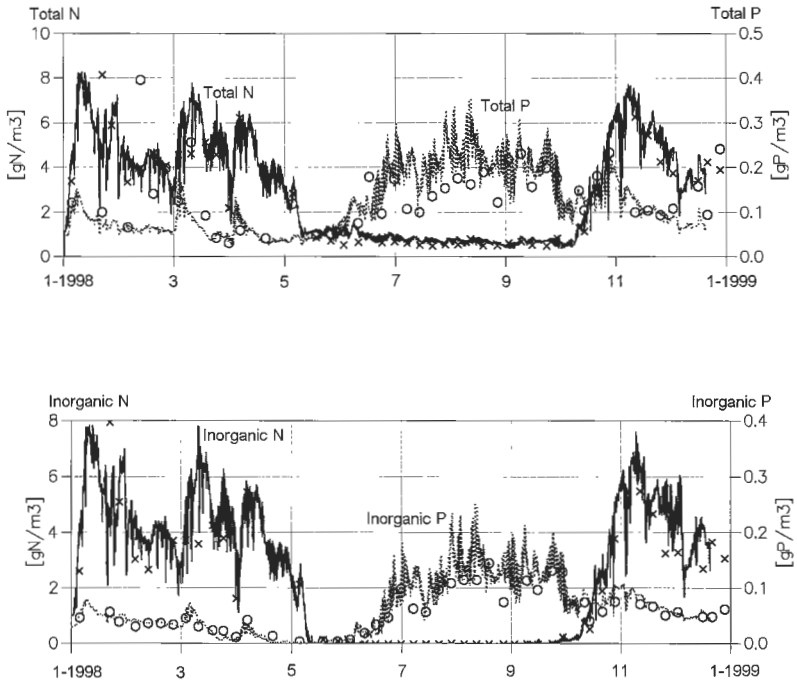


Figure 6 *Simulated and measured concentrations in Odense Fjord of total N & P (top panel) and inorganic N & P (lower panel).*

The sediment module was tested on Odense Fjord, RASMUSSEN et al. (2000), as previously mentioned. The effects of the sediment in Odense Fjord

on the water quality were very pronounced in some periods. The effects were intensified in Odense Fjord compared to what would be expected in, for example, the Southern part of the Kattegat, which is mainly due to large areas of very shallow water. Because the same processes take place in the two localities, a sediment module tested and verified on Odense Fjord is also expected to be capable of describing the sediment dynamics in the Southern part of Kattegat. In addition, the credibility of the sediment model is increased when the model reproduces the concentrations of the different components in the water column in a system such as Odense Fjord where the sediment dynamics periodically regulates the water quality, Figure 6.

It would not have been possible to reproduce the release of phosphorus in particular during the summer period resulting in high phosphorus concentrations in the water. By introducing the sediment module it is possible to make a complete mass budget of the fjord including the different components in the sediment.

3 RIVER RUNOFF

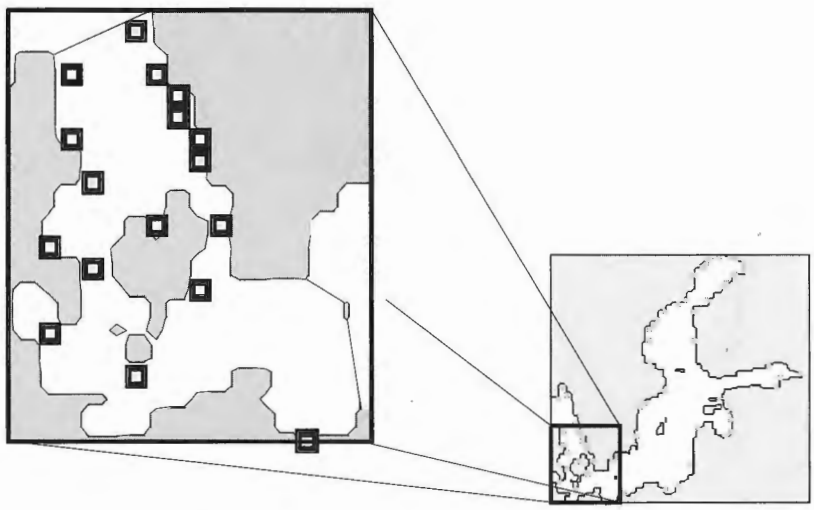


Figure 7 Rivers included in the SCOBI 3D model

Daily river runoff is estimated by the Swedish hydrological HBV-Baltic model, GRAHAM (2000). The HBV-model is a large-scale model that covers the entire Baltic drainage basin. In the HBV-Baltic model, the entire Baltic-Kattegat-Skagerrak drainage area is divided into 43 hydrological sub-basins. Those sub-basins represent the drainage basins for the Baltic Sea coastal areas, following the SVAR (Swedish Water Archive) Sea Area Register. Eight of those sub-basins cover the drainage area of the modelled Kattegat-Arkona area.

Seventeen of the largest rivers in the Kattegat-Arkona area are taken into account within the Kattegat-Arkona model set-up, Fig. 7. Using a 20-year climatological estimate of the river run-off for each separate river, the simulated river run-off from the eight HBV-Baltic sub-basins is distributed to

the rivers. The climatological river run-off also serves as a fallback in case there are no HBV-Baltic data available.

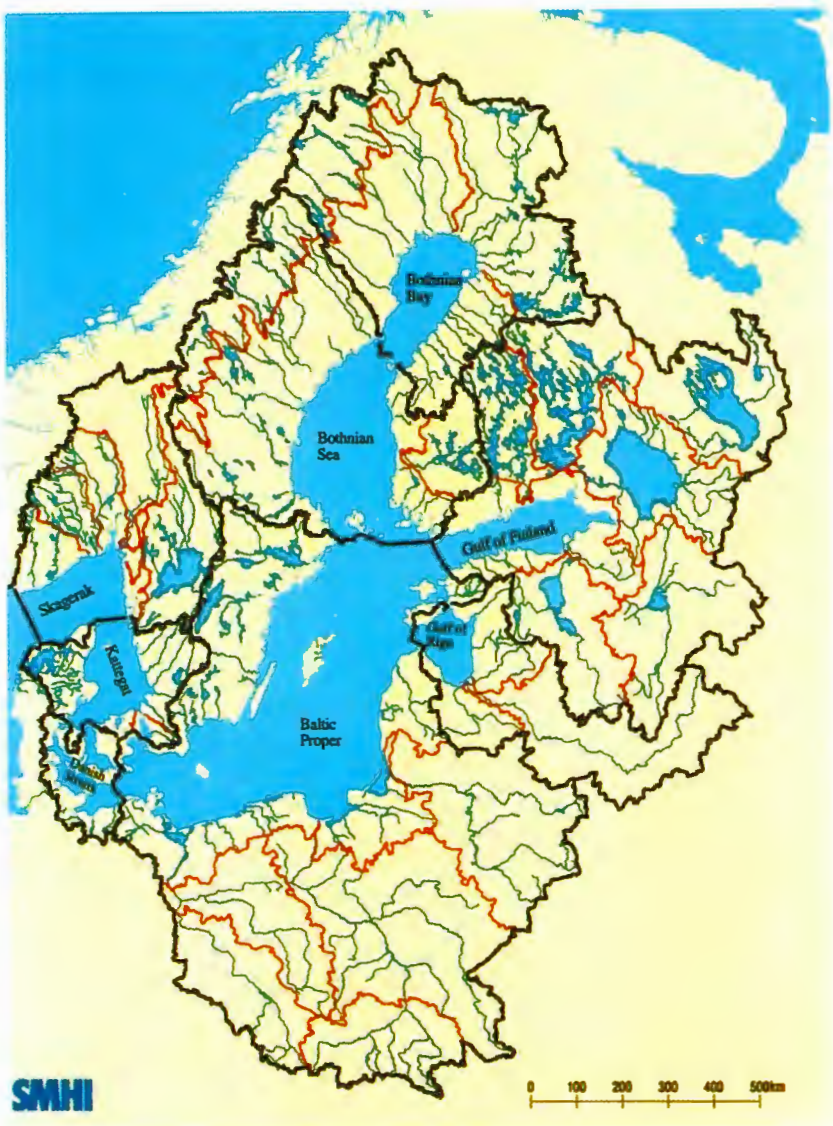


Figure 8 *Subbasins of the riverine HBV-N model, where the black line indicates the subbasin of the chemical model and the red lines indicate the subbasin of the water transport model*

The continuous riverine nitrogen transport model, HBV-N, has been coupled to the integrated model system, MARMEFELT et al. (1999), PETTERSSON et al. (2000) and ARHEIMER and BRANDT (1998). The HBV-N model has been set up for the entire Skagerrak-Kattegat-Baltic drainage, excluding the river Göta älv. The HBV-N covers 29 sub-basins around the Baltic; four of them cover the Kattegat-Arkona area, Fig. 8. Unfortunately, the HBV-N model has only been run for the period of 1980 – 1994. So at present, we use the 13-year climatological estimate for the nitrogen concentration, STÅLNACKE (1996), that only will serve as a fall back for the modelled nutrient data in the future, for the Swedish rivers and available data from the Danish rivers. But

nevertheless, the model system has been set up so that the HBV-N data will be used as soon as they become available.

A riverine phosphorous model is under development at the SMHI and will be implemented to the model system as soon as possible. For the time being, however, Stålnacke climatological data has been used for the Baltic phosphorous riverine load, and available Danish data for the Danish rivers.

4 ATMOSPHERIC DEPOSITION

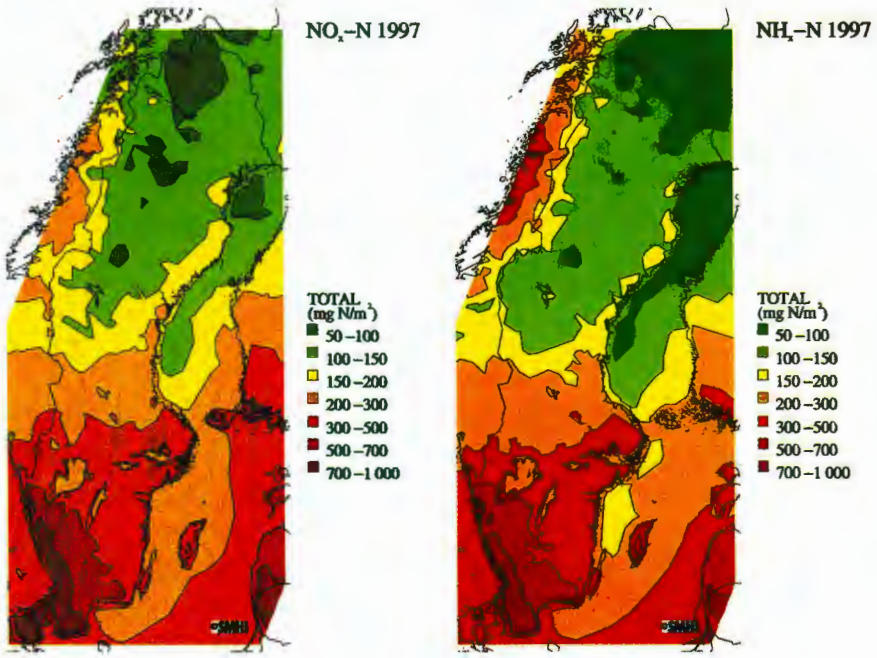


Figure 9 *Annual deposition of NO_x and NH_x during 1997, calculated by the MATCH model.*

The atmospheric input of oxidised and reduced nitrogen is taken from the annual assessments carried out with the MATCH-Sweden modelling system developed at SMHI, LANGNER et al. (1995). MATCH-Sweden combines model calculations, using an atmospheric transport and chemistry model, with observations of air- and precipitation chemistry data and meteorological conditions to estimate the deposition of nitrogen compounds over Sweden.

During the development of the MATCH-Sweden model system, focus has been on the deposition over land and not the Baltic Sea itself. Up to now, the MATCH-Sweden therefore only covers parts of the Baltic drainage area with its 20×20 km horizontal resolution, Fig. 9. Instead of using the MATCH-Europe model for the area outside the MATCH-Sweden modelling area, in this project we have chosen to simply mirror out the deposition data outside the modelling area. The reason for this rudimentary treatment of the atmospheric deposition is that we have chosen to focus on a running integrated model

system and await for the MATCH-Sweden modelling area to be extended to cover the whole Baltic drainage basin, as it will be in the near future.

5 OPEN BOUNDARY

To avoid problems with the open boundaries to the area, the SCOBI-3D has been set up for the entire Baltic-Kattegat-Skagerrak area. The only open boundary we have to deal with will be towards the North Sea. The open boundary is situated between Kristiansand in the north and Hanstholm in the south.

Monthly monitoring of oxygen, nitrate, phosphate and chlorophyll is carried out by the Institute of Marine Research in Norway at a cross-section between Torungen in Norway and Hirtshals in Denmark. The available data is treated as boundary values at the open boundary. Remaining model variables, for which monitoring data is not available, a no-flux condition is set at the boundary simply by mirroring out data from the model area. Although this is not a perfect solution, we hereby ensure us that we don't import 'strange' values into the model. This is only a temporary solution, as the SCOBI-3D model will be coupled to the Norwegian NORWECOM-model for exchange across the open boundary in the ongoing project NO COMMENTS, which is financed by the Nordic Council of Ministers.

6 RESULTS AND VALIDATION

In several aspects, 1997 was an extraordinary year for the Baltic-Kattegat-Skagerrak area. The spring bloom in the Skagerrak-Kattegat area, for example, was extremely early. It was fully developed already when the Swedish monitoring cruise was carried out in late January. Normally the spring bloom in the area takes place in late February or early March, a few days earlier in the Skagerrak compared to the Kattegat. In 1997, it was like the autumn bloom never ceased. The summer temperature was the highest that had been observed in the southern part of Sweden during the 20^{th} century, which of course affected the sea surface temperature in the Baltic Proper. A temperature record of 24°C was observed in the surface layer in central Baltic Proper. The third extreme event that took place during 1997 was a massive flooding from the Polish rivers Odra and Wisla in July, BRANDT et al (1998), due to massive precipitation in Poland and the Czech Republic. However, one were not able to detect any effects on the open sea near the Gdansk Bay or Pomeranian Bay during the cruises carried out at the time. The main reason was that the flooding occurred during the production season, and that the extreme land load of nutrients was consumed very close to the coast.

In this aspect it is quite a challenge to simulate the biogeochemical cycle of 1997. But maybe it is to have far too high expectations to think that the prototype model system in its first application should be able to catch all these extreme events especially with this version of a coarse horizontal grid of 12 nm that the model is reduced to.

6.1 INITIALISATION

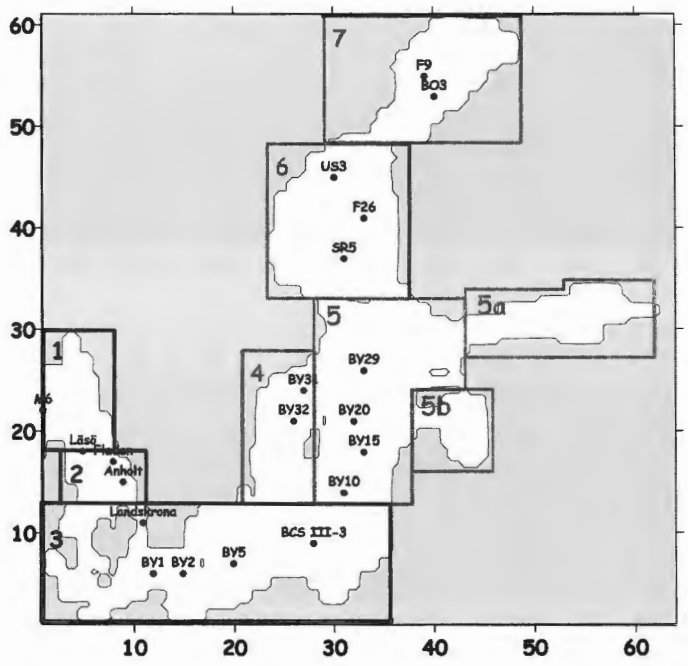


Figure 10 *The sub-areas for the initialisation of the SCOBI model in the Baltic Sea-Kattegat-Skagerrak area.*

To start with, the SCOBI-HIROMB model has to be initialised. For the hydrodynamic part, a model field from a previous forecast was used as initialisation. The HIROMB model was started in October 1996 and run for 2 months for spin-up. Thereafter monitoring data were used for those SCOBI variables that are included in the monitoring program. For remaining variables (zooplankton, detritus and the benthic pools) a low winter value was chosen.

The entire model area was divided into seven main sub-areas, Fig. 10, with respect to cross-section made from available monitoring stations. The Baltic Proper sub-basin has been divided in three, because the Riga Bight and the Gulf of Finland actually differs from the Baltic Proper, but we suffer from a lack of data. The initial values for the Gulf of Finland and the Riga Bight are taken from the Baltic Proper except for the surface layer were we have used typical Riga Bight winter values of nitrate (15 μmol l^{-1}) and phosphate (0.8 μmol l^{-1}).

Fig. 11 shows a cross section from the Skagerrak through the Baltic Proper passing east of the Gotland Basin to the Bothnian Bay. Chlorophyll is only monitored in the upper 20 m. Initial values are therefore set to 0 below 20 m in the model. No monitoring data of chlorophyll are available for the Gulf of Bothnia, but we have chosen a low concentration winter value of 0.1 μg-chl l^{-1}. For the Gulf of Bothnia oxygen concentration we had to assume oxygen saturation in the surface layer as oxygen is only monitored at the bottom in the Gulf. Below the surface layer we assumed a linear declination towards the monitored bottom values.

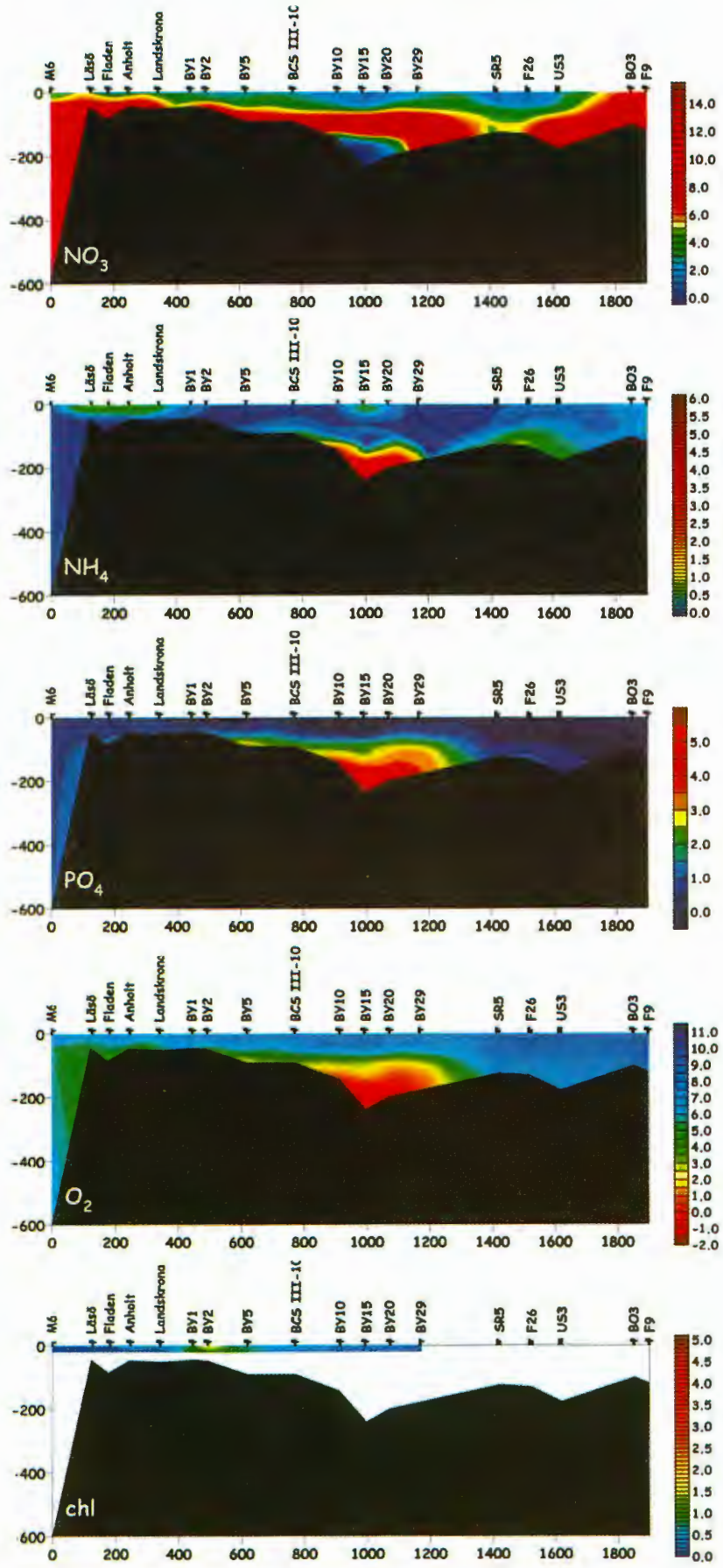


Figure 11 *Cross-section from the open boudary in the Skagerrak through the Kattegat, the Baltic Proper east of Gotland Island and ending in the Bothnian Bay of monitoring data carried out in December 1996*

6.2 Model Results

As the SCOBI-3D model has been run for the entire Skagerrak-Kattegat-Baltic region, results from the entire region will be presented in this section. The validation in the next section, however, will be concentrated to the Kattegat-Arkona region. The model results presented here are focused on surface distribution of plankton, nutrients and detritus concentration together with bottom oxygen concentrations. The discussion of the model results is mainly focused on whether the SCOBI-3D model is able to simulate the biogeochemical annual dynamics correct in time and space and whether the simulated concentrations are of right magnitude.

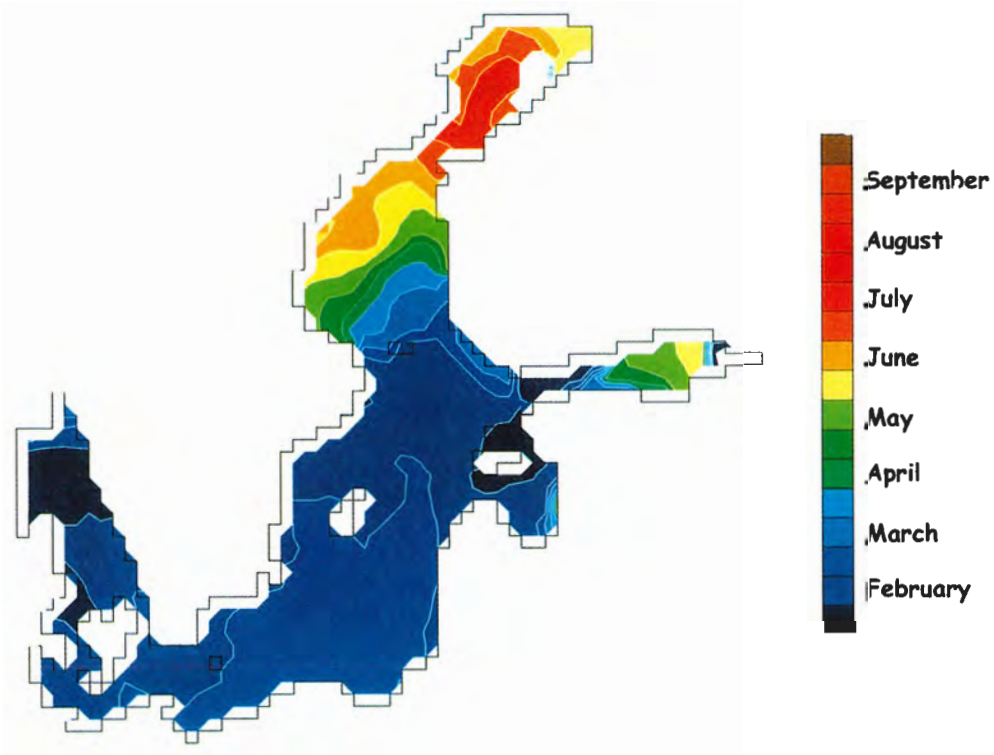


Figure 12 *The spring bloom in the SCOBI model starts in the Skagerrak and in the entrance to the Gulf of Finland and is spread southwards. Once established in the Baltic Proper it is spread northwards into the Gulf of Bothnia.*

Fig. 12 illustrates the on set of the spring bloom in the model, were it is shown that the simulated spring bloom begins in the Skagerrak-Kattegat area a few weeks earlier than in the Baltic Proper. When the spring bloom starts in the Baltic Proper it firstly develops in the northern part and eventually it is spread southwards. In late spring/early summer the spring bloom starts in the Bothnian Sea and finally it reaches the Bothnian Bay. The dynamics of the spring bloom in the model follows the generally pattern of what is known from observations. However, the extremely early spring bloom in the Skagerrak-Kattegat area that occurred in 1997 is, as will be seen in the validation below, not caught in the model. In reality the spring bloom was fully developed in January, but in the model it has only started to develop at that time. The simulated spring bloom in the Skagerrak-Kattegat area is not fully developed until late February as will be shown in the validation section below.

To a large extent, the biogeochemical processes are governed by the hydrodynamics in the ocean. To a large extent, the prevailing circulation explains the spatial distribution of the biogeochemical parameters. In Figs. 13-30 biweekly model output for the surface layer is shown for the different model variables. The sharp front of the northward spreading of the Bothnian Sea spring bloom that is shown in Fig. 25, is an example of how the circulation affects the biogeochemistry in the area. In this case, currents from the north prevent the autotrophs from spreading northwards.

The sharp plume of the modelled autotrophs, Figs 25-26, and detritus, Figs. 29-30, that is found at the outlet of the rivers Gide älv, Ångermanälven, Indalsälven and Ljungan in the Bothnian Sea is mainly due the model formulation of their sedimentation. Adding the fact that the circulation in the area is rather modest and that the riverine nutrient supply is high, the high concentrations produced by the model is explained. A sharp plume of modelled zooplankton concentration, Figs 27-28, is also present at the same location. In the model the zooplankton emerges were food is available. In the autumn, when the production season ceases, the model, Figs. 22 & 24, produces nutrient plumes at this special location. These plumes explained by intense mineralisation in combination with low photosynthetic production and the land load.

For the same reason, same pattern is found northweast of the Gotland Island with high concentrations of autotrophs, Figs 25-26, and detritus, Figs. 29-30, captured between the Swedish mainland and the Gotland Island. This is more agreeable with what is known from observations, although the concentrations are twice as high as the chlorophyll concentration being recorded. One reason for the high chlorophyll concentrations in late summer is that the SCOBI model only accounts for a fixed C:chl ratio of 50:1. In reality, the biomass during the secondary bloom is usually high, while the chlorophyll content in the cells is low. To fully account for this effect, it should be necessary to introduce a variable C:chl ratio in the model. Another reason is that we in this project have adjusted the sedimentation of the phytoplankton and the detritus so that the sedimentation velocity is reduced when the stratification is high. It is well known that a massive accumulation of both phytoplankton and detritus can be found in a thin layer at the pycnocline. As we have been focusing on the Kattegat-Arkona area with its sharp stratification the reduction of the sedimentation rate in the pycnocline has been formulated mainly to fit strongly stratified waters. For the time being, we have to be satisfied with the fact that the present formulation of the sedimentation works well in the Kattegat-Arkona area, and that more careful calibration is needed until the sedimentation is well functioning also in water with less pronounced stratification.

Following the annual nutrient dynamics, Fig. 19-24, the season begins with high nitrate and phosphorous concentrations in the surface layer. The ammonia concentrations are much less except for in the Kattegat. As the spring bloom starts the inorganic nitrogen is consumed. The phytoplankton prefers ammonia to nitrate, so as long as ammonia is available ammonia is consumed. As soon as the ammonia pool in the surface layer is emptied, the phytoplankton turns

towards the nitrate for assimilation. It is also noticeable that once the spring bloom has started, and the nitrate concentrations turn low, the bloom is maintained by the external supply of inorganic nitrogen. For the Baltic Proper phosphorous cycle is a bit different. West of the Gotland Island the model produces high phosphorous concentrations in the surface layer during the spring bloom. At the end of June, when the system is depleted of nitrate, the nitrogen fixation starts and phosphorous is consumed. In mid September the nitrogen fixation reduces and the phosphorous pool is regained. This annual cycle west of the Gotland Island is well known from monitoring data.

A general problem that we have with this coarse model set up of 12 nm resolution is to keep the stratification. The horizontally averaged salinity and temperature has been adjusted with ordinary nudging to the model field from the one-dimensional model PROBE-Baltic every time-step. The PROBE-Baltic is a coupled 13-basin model that runs operationally at the SMHI. For the nudging, the HIROMB model area has been divided into 13 sub-areas to fit the PROBE basins. The nudging has thereafter been carried out within the 13 areas separately.

With the help of the nudging procedure, the salinity and temperature fields are kept realistic. The problem with coupling a biogeochemical model to a hydrographical model that need *'artificial help'* for keeping proper hydrographical fields, is that the biogeochemical variables will be transported by the model's internal physics. The biogeochemical variables are not affected by any nudging. Some of the shortages in the SCOBI-3D model are a direct result of the shortages in the hydrodynamics of the coarse resolution of the 12nm HIROMB model. For example is it difficult to keep low oxygen concentrations in the deep waters of the Gotland basin (east of the Gotland Island), Figs. 31-32, because difficulties with simulating the dense bottom current properly. Well-oxygenated water is transported into the basin much more frequent in the model than what has been observed. Also the winter convection of nutrients that starts after the production season and supplies the surface layer with high concentrations of nutrients during winter will be affected as the nutrients in the deepwater is mixed and the nutricline becomes less pronounced or even totally vanishes.

These effects are reduced by increasing the horizontally and vertically resolution, which will be the next obvious step in the near future model development in addition to the improvement of the mixing parameterisation.

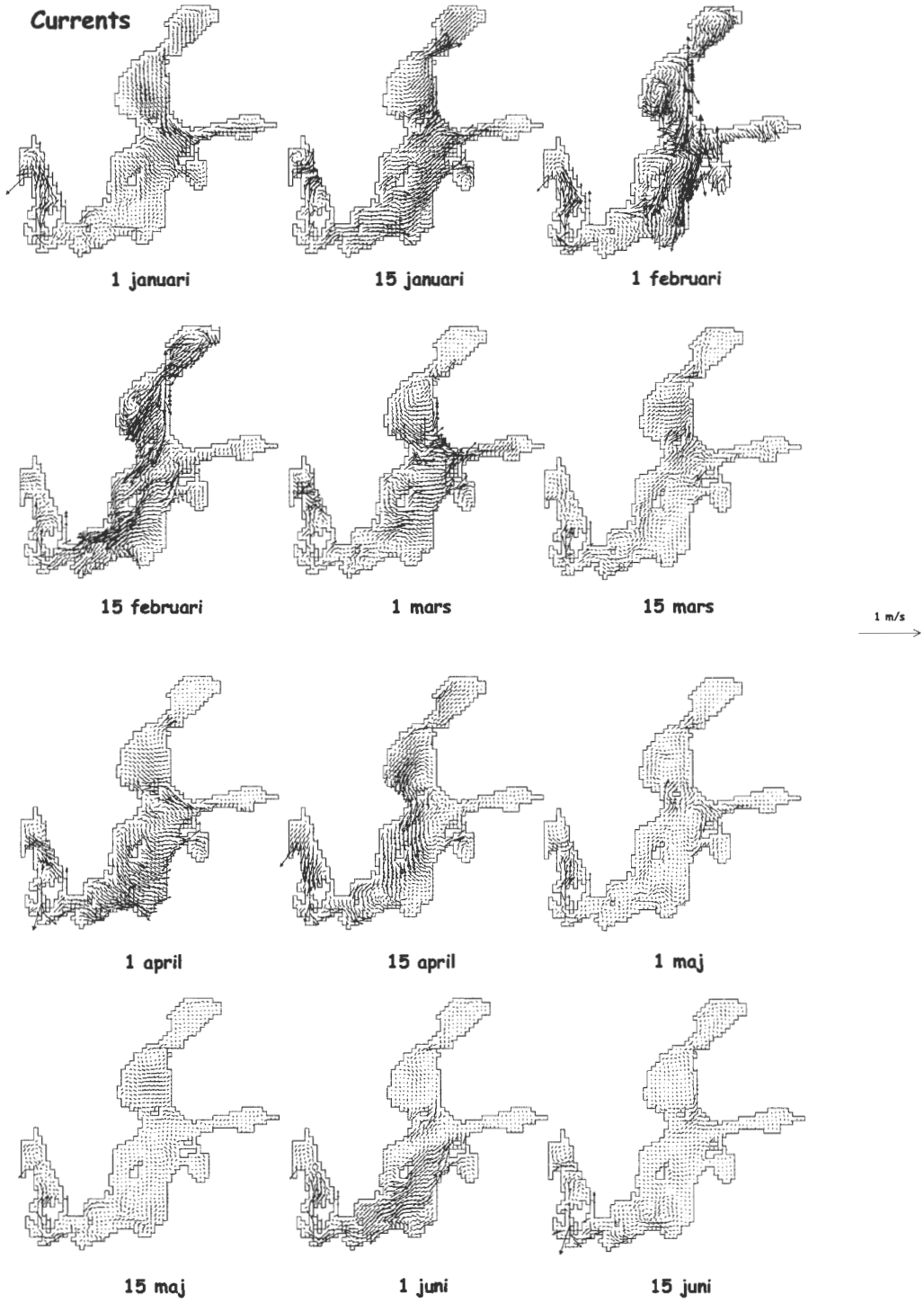


Figure 13 *Biweekly simulated currents in the surface layer during January – June 1997*

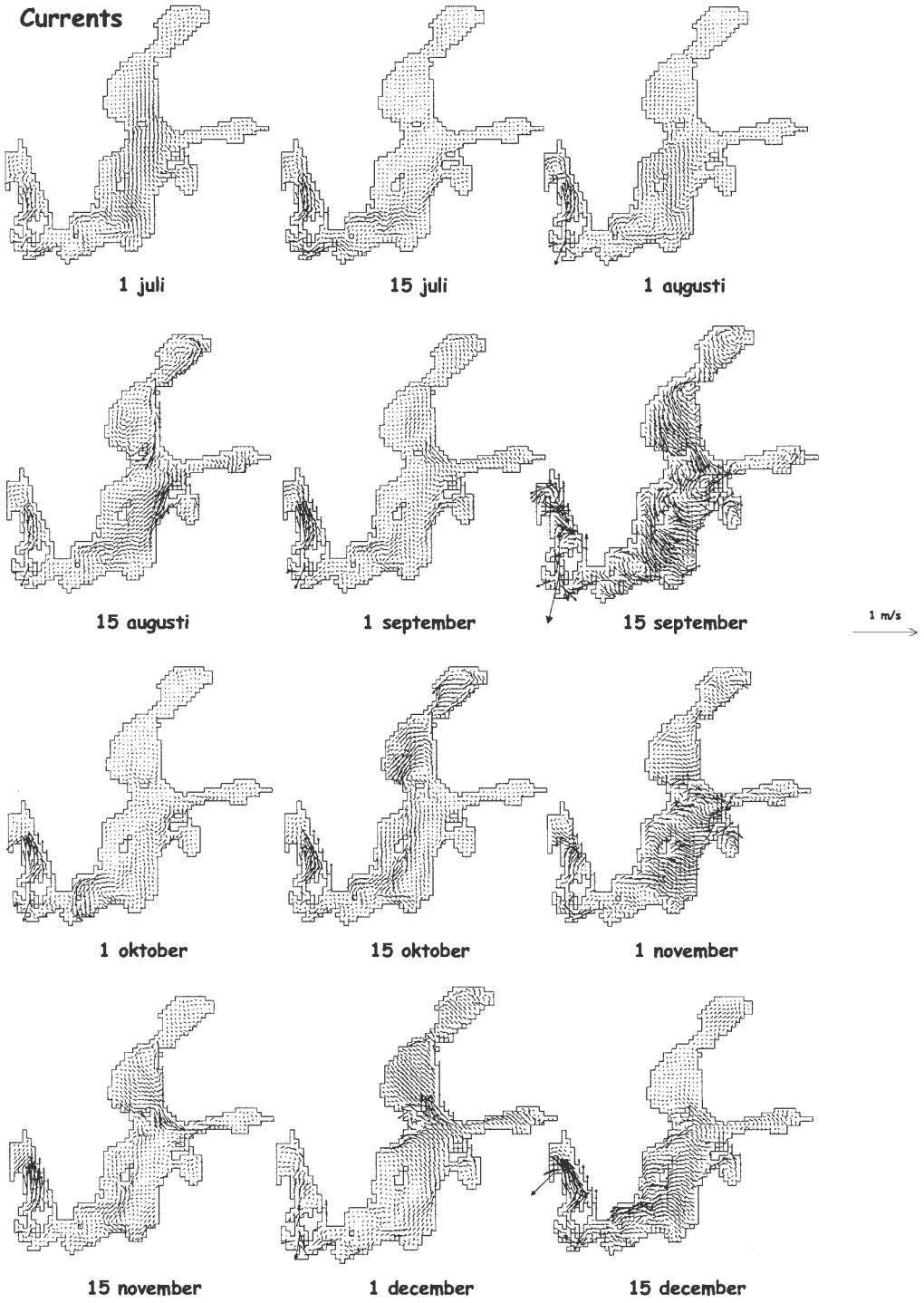


Figure 14 *Biweekly simulated currents in the surface layer during July – December 1997*

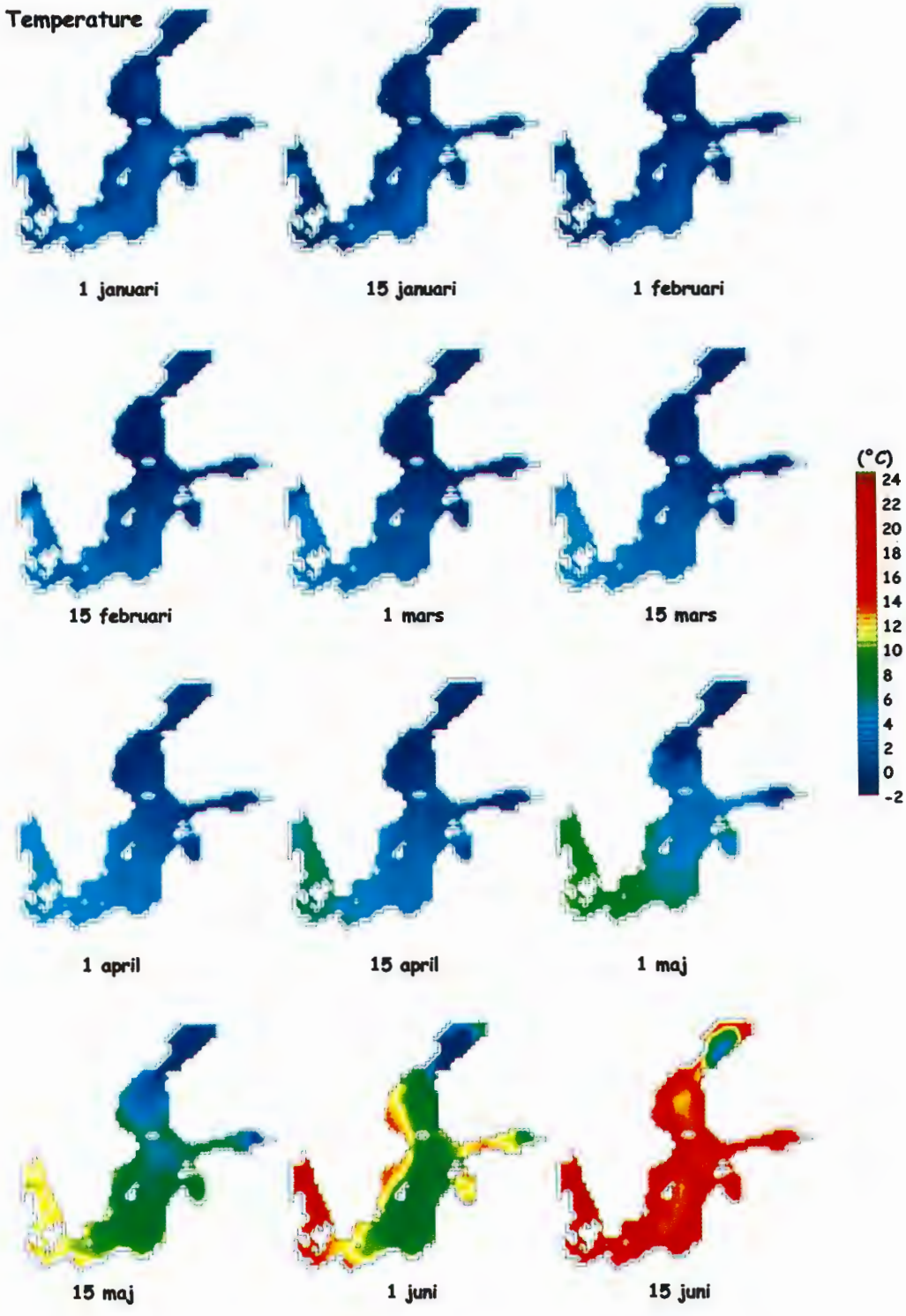


Figure 15 *Biweekly simulated temperature in the surface layer during January – June 1997*

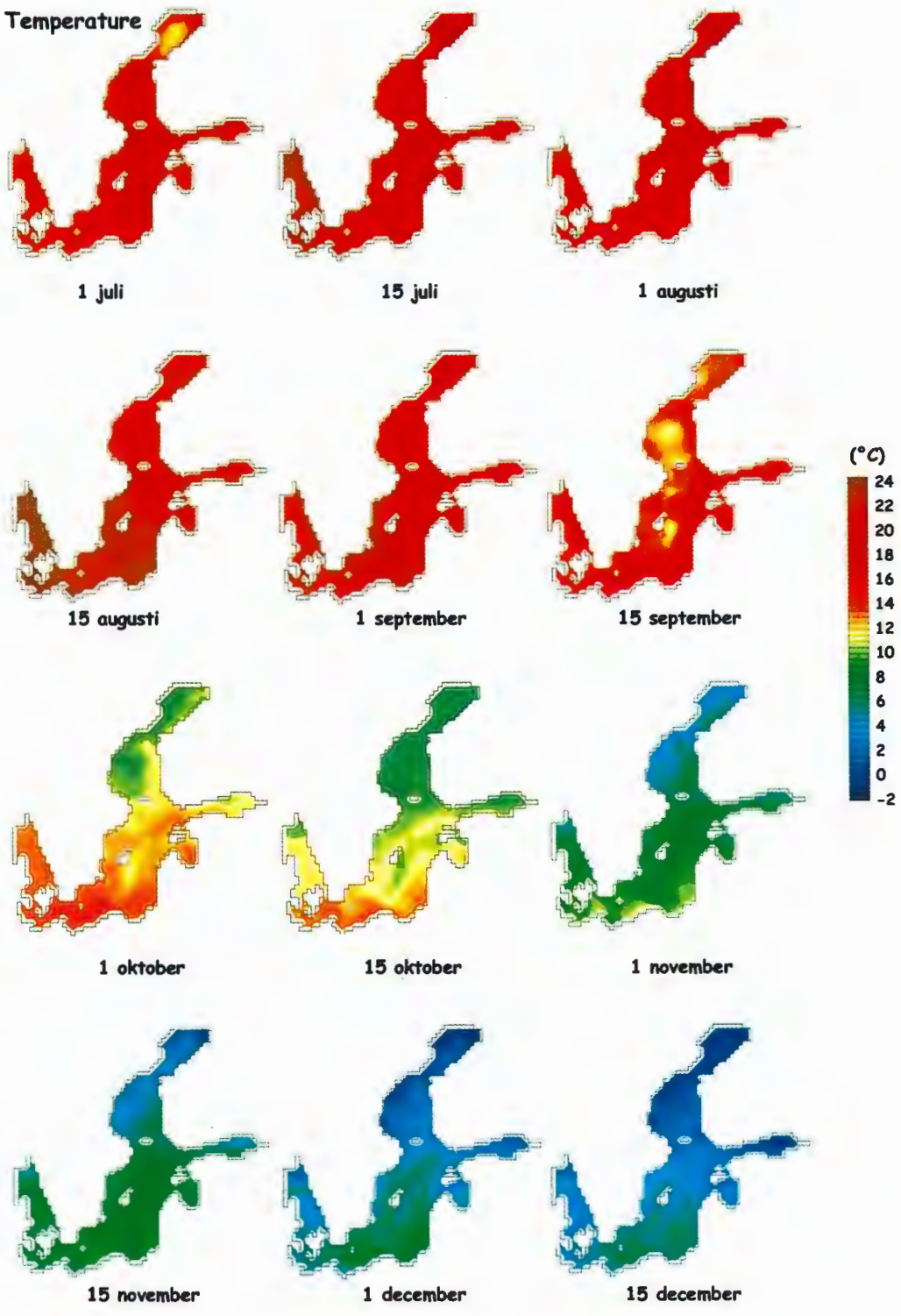


Figure 16 *Biweekly simulated temperature in the surface layer during July – December 1997*

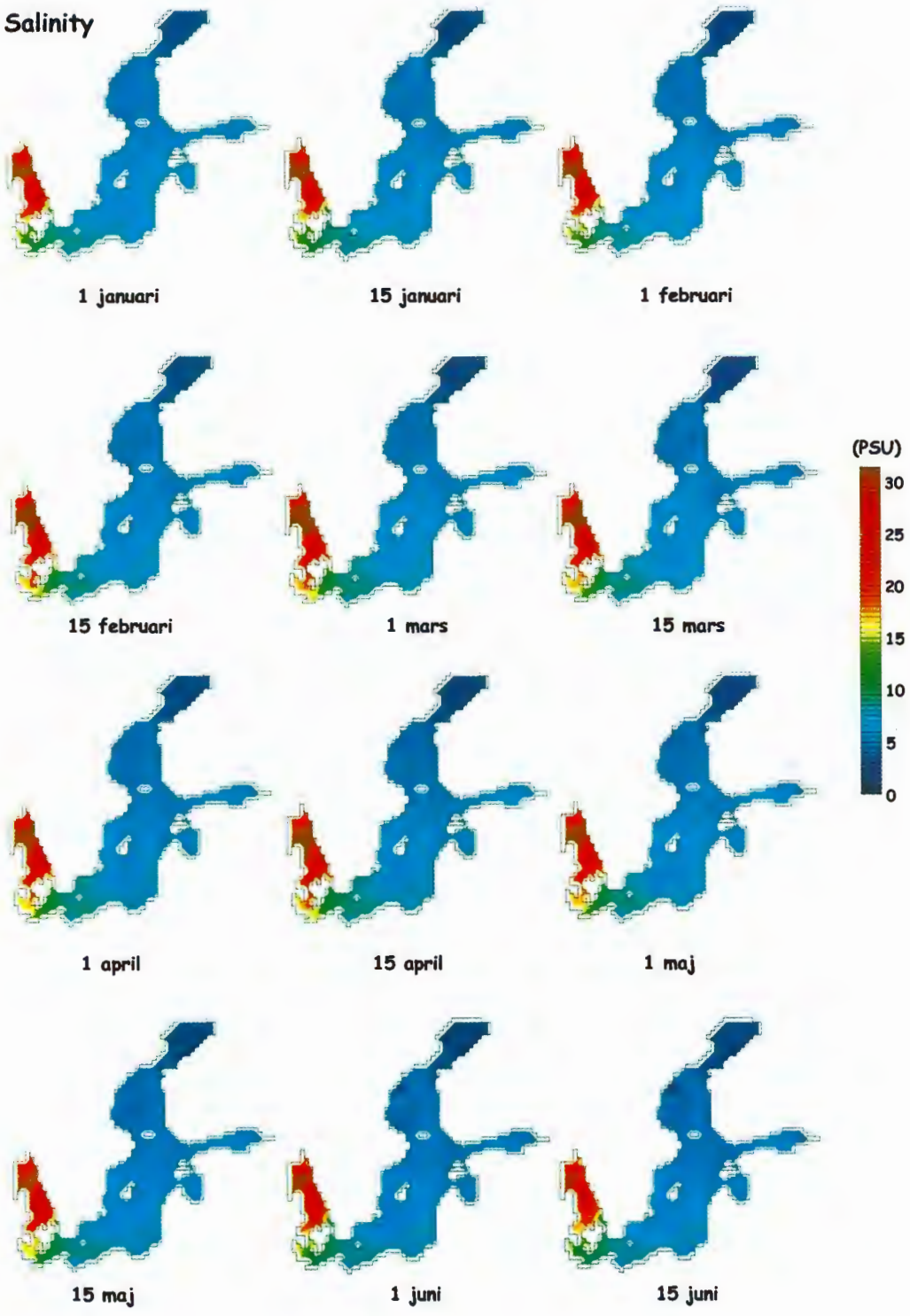


Figure 17 *Biweekly simulated salinity in the surface layer during January – June 1997*

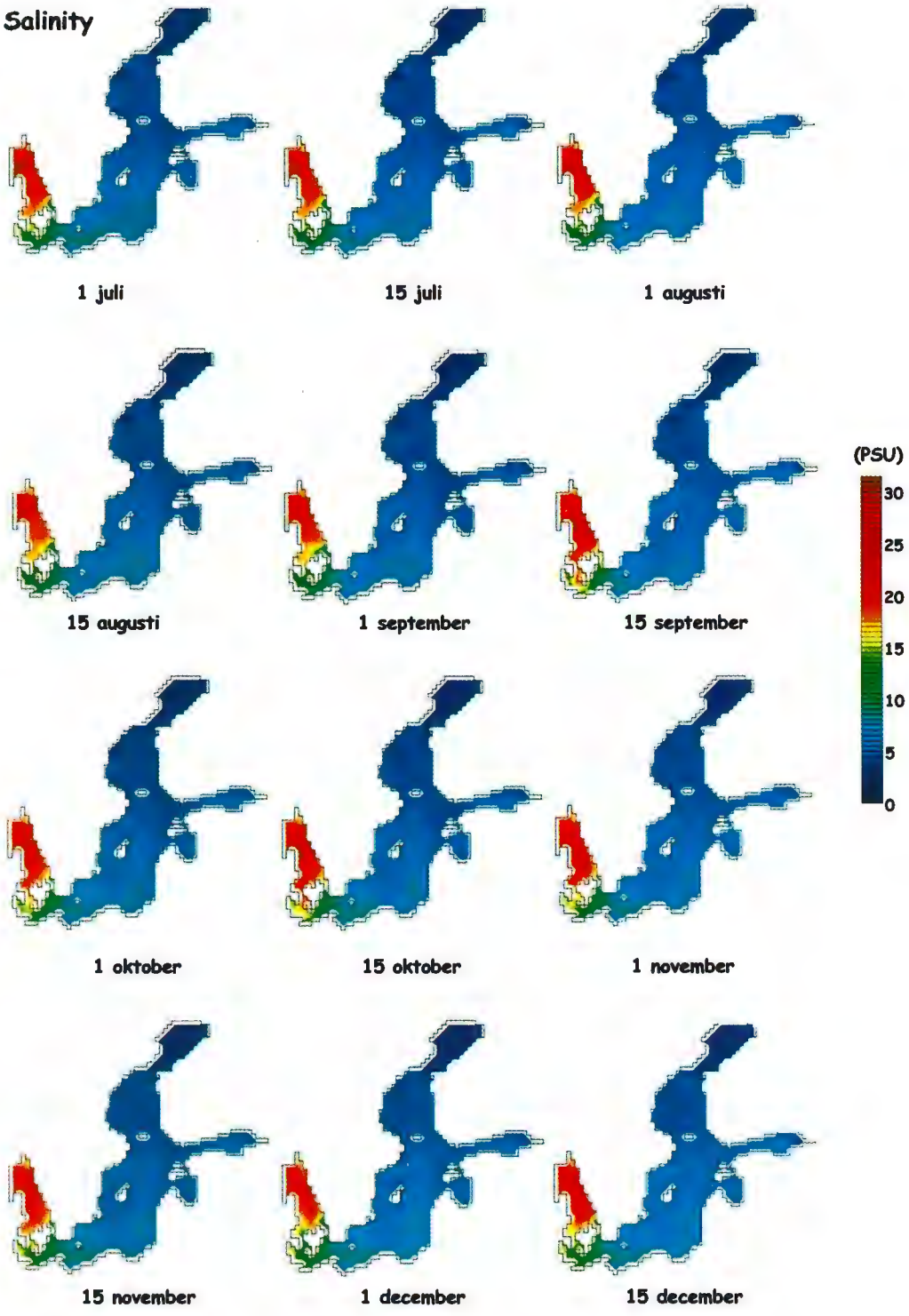


Figure 18 *Biweekly simulated salinity in the surface layer during July – December 1997*

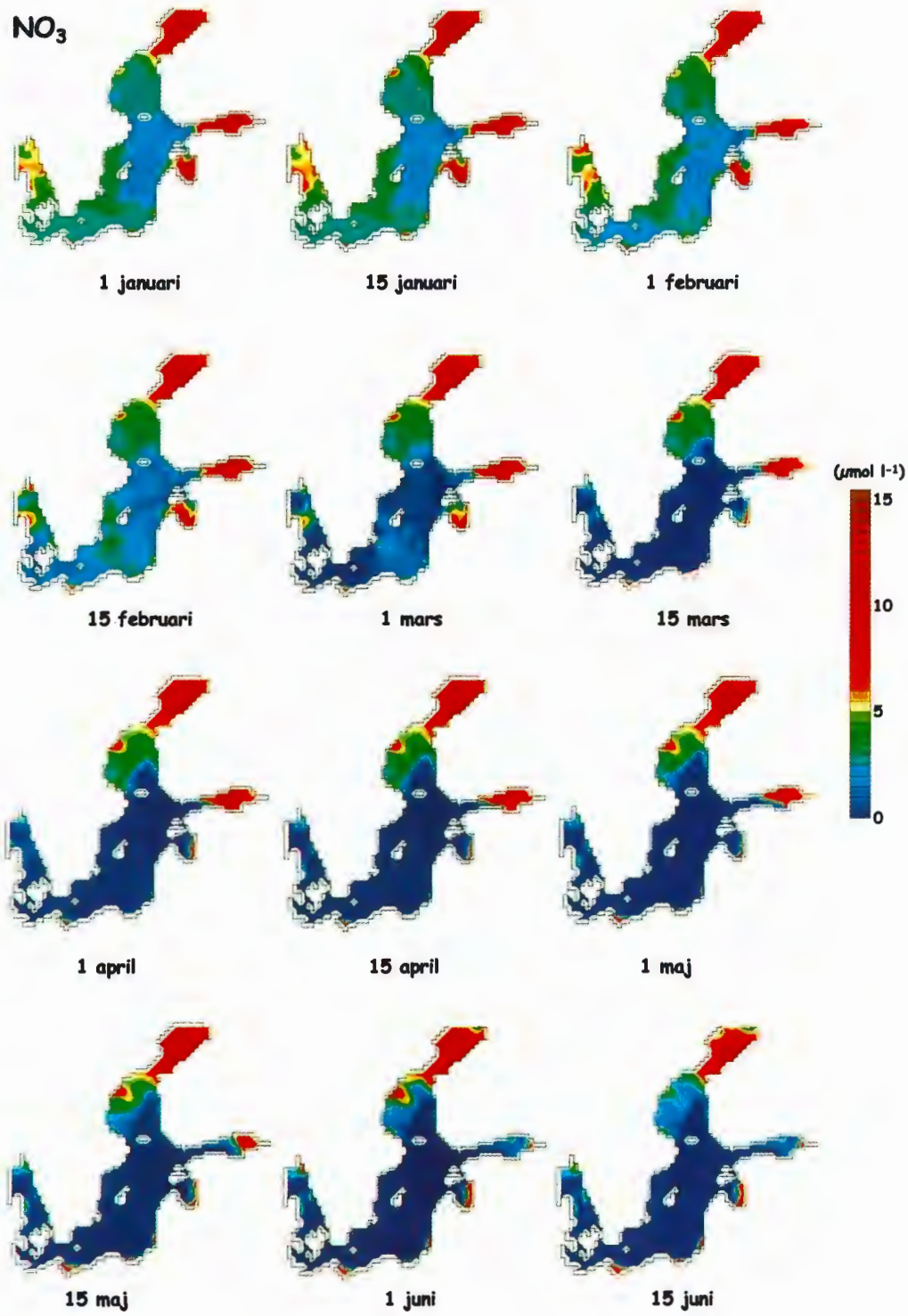


Figure 19 *Biweekly simulated nitrate concentrations (µmol l^{-1}) in the surface layer during January – June 1997*

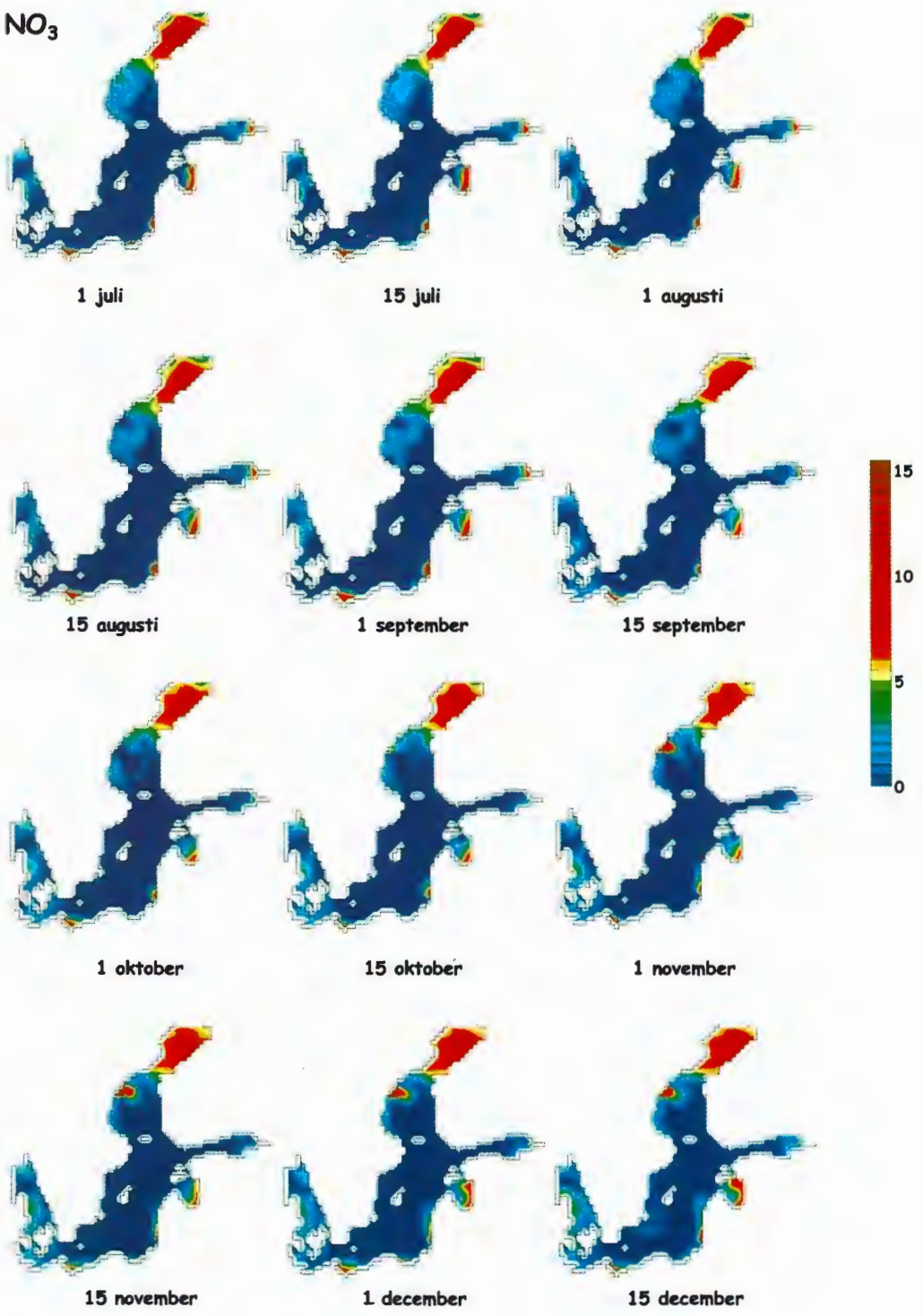


Figure 20 *Biweekly simulated nitrate concentrations (µmol l^{-1}) in the surface layer during July – December 1997*

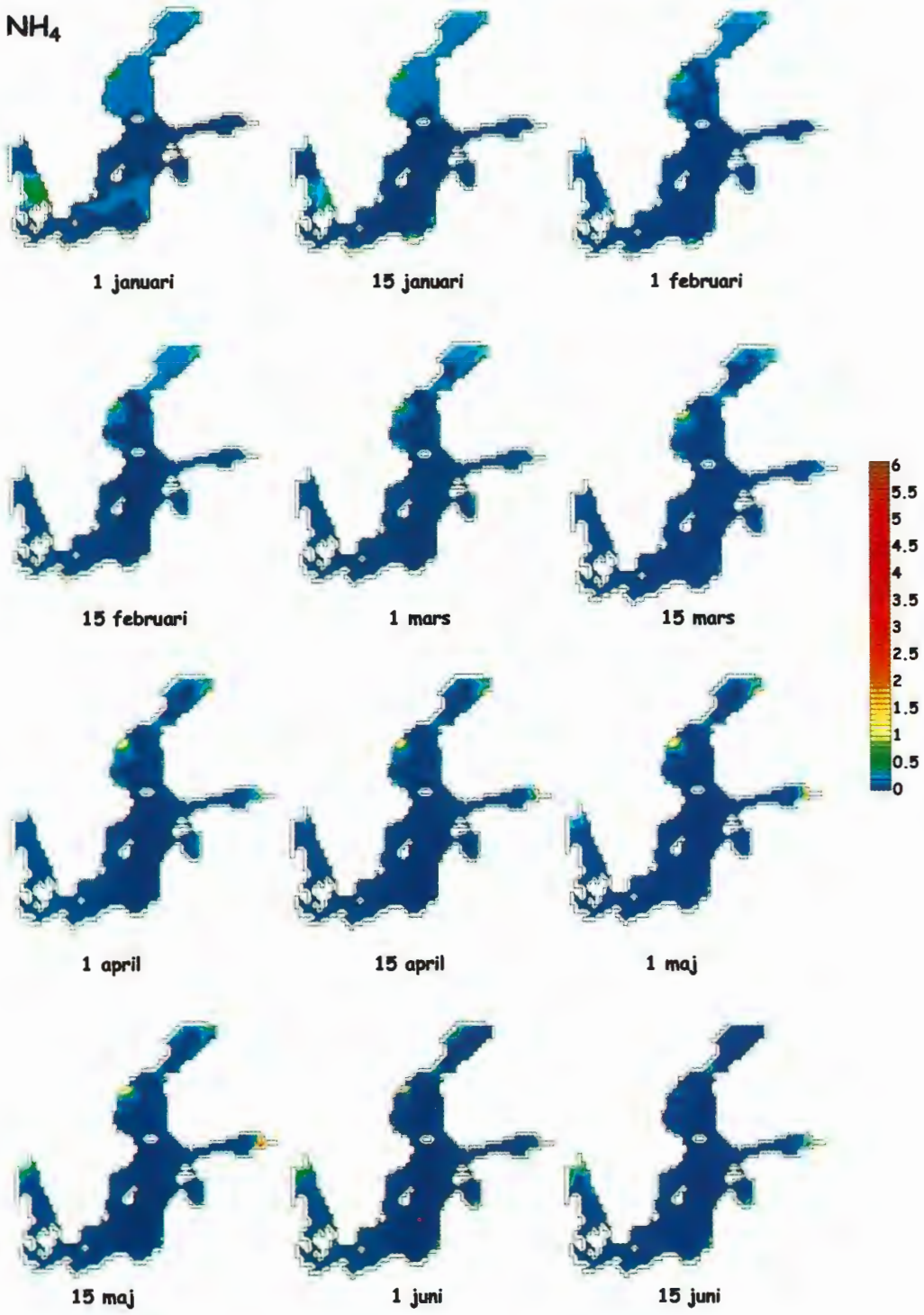


Figure 21 *Biweekly simulated ammonia concentrations (µmol l^{-1}) in the surface layer during January – June 1997*

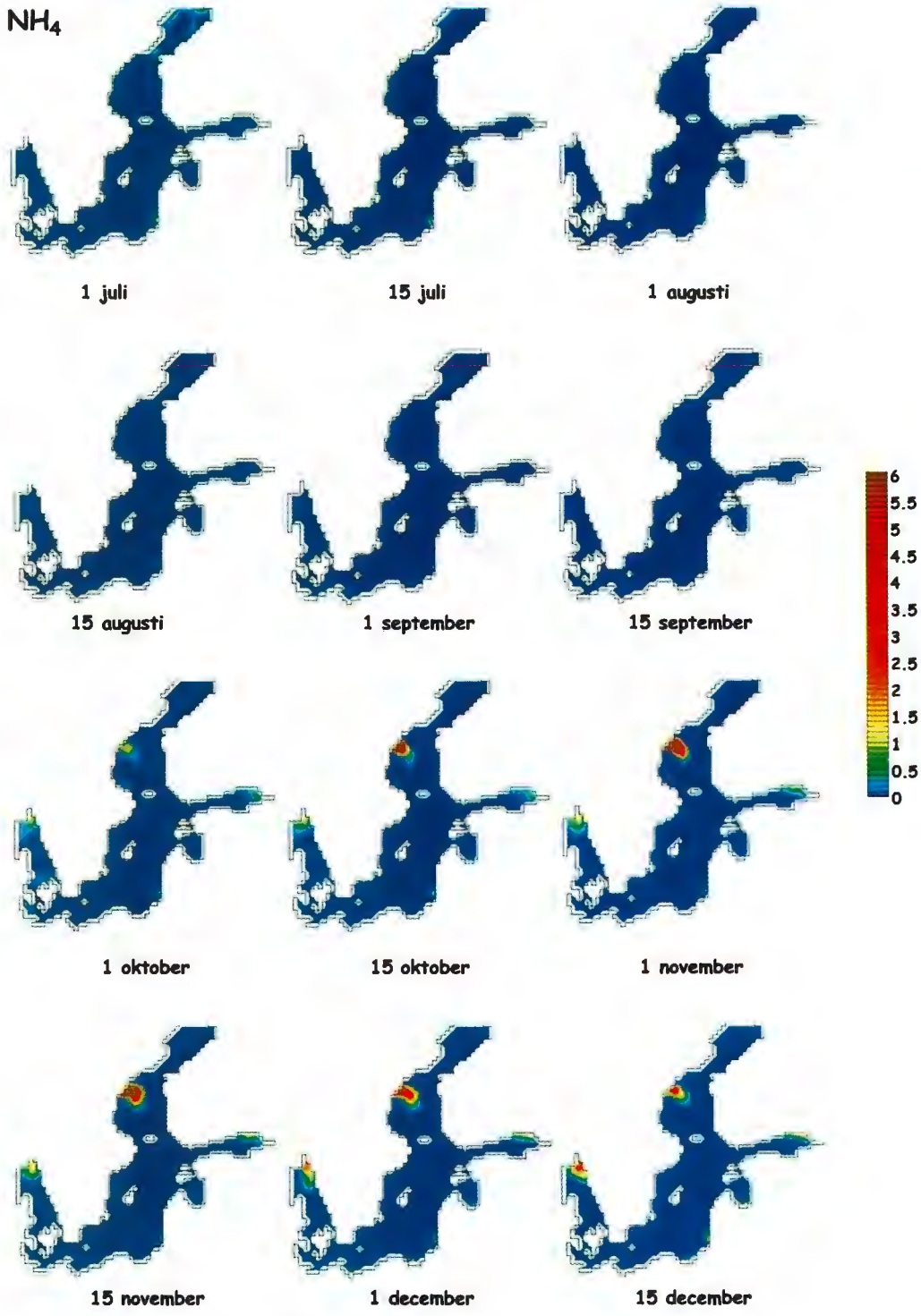


Figure 22 *Biweekly simulated ammonia concentrations (µmol l^{-1}) in the surface layer during July – December 1997*

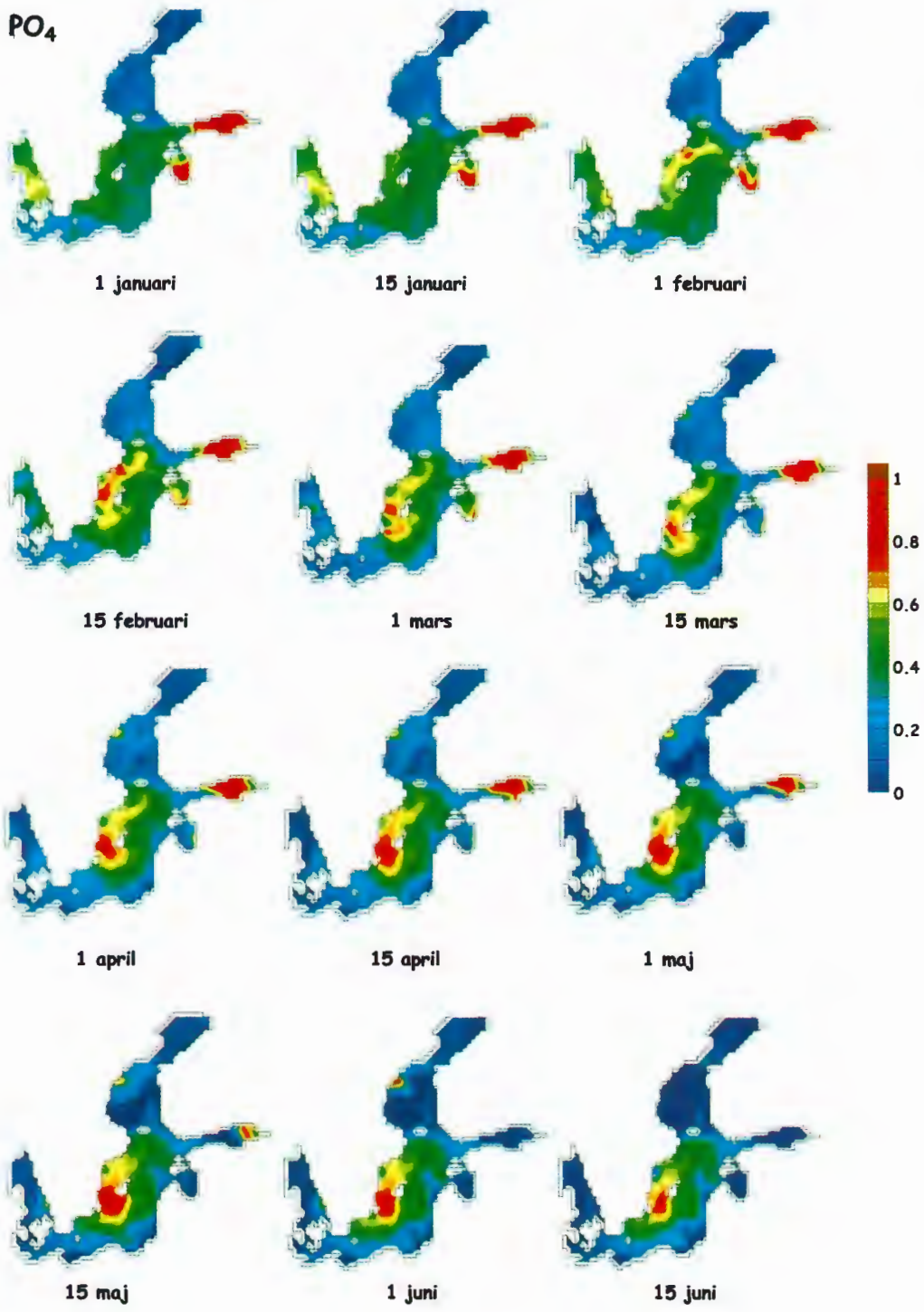


Figure 23 *Biweekly simulated phosphate concentrations (µmol l^{-1}) in the surface layer during January – June 1997*

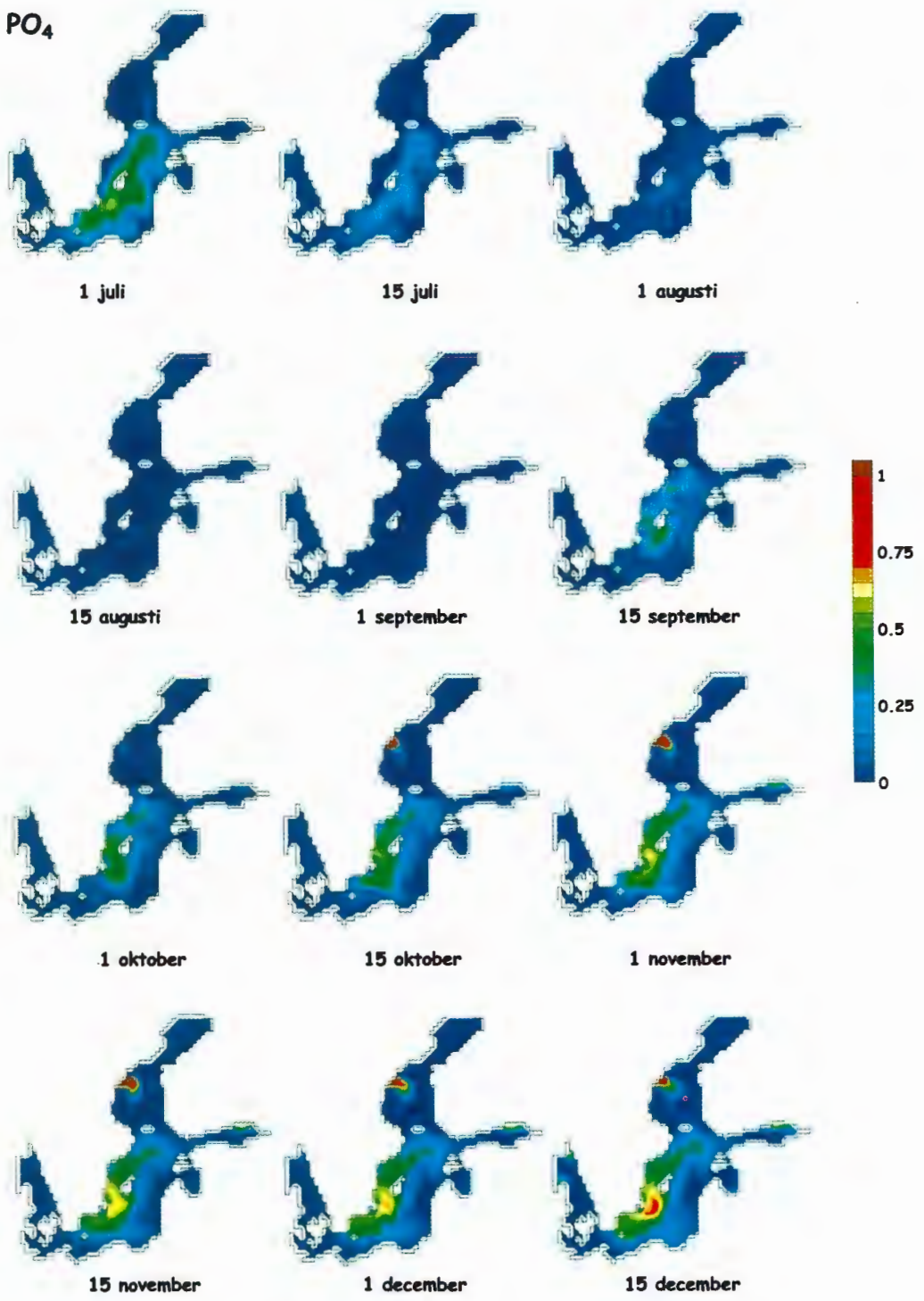


Figure 24 *Biweekly simulated phosphate concentrations (µmol l^{-1}) in the surface layer during July – December 1997*

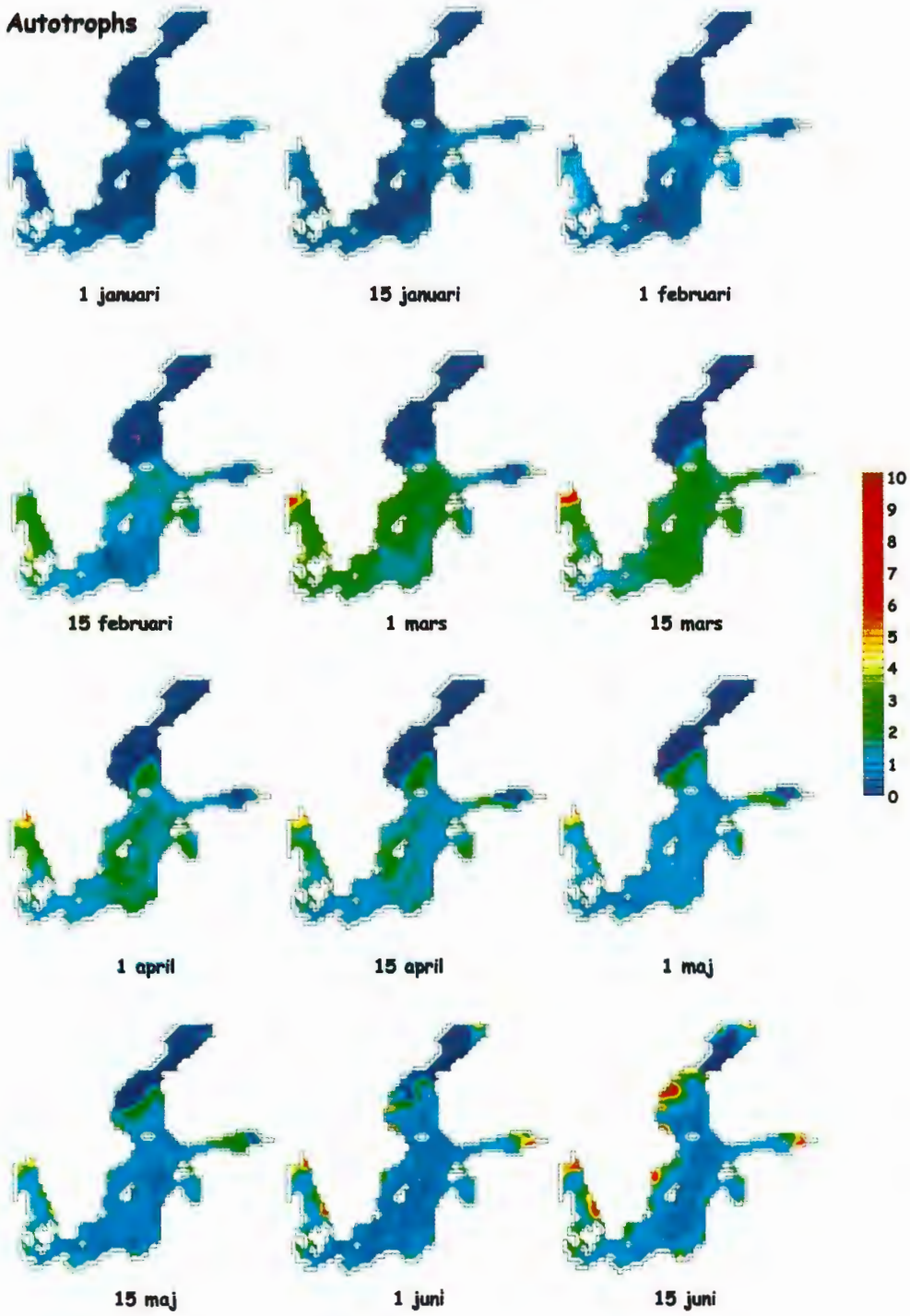


Figure 25 *Biweekly simulated autotroph concentration (µg chl l^{-1}) in the surface layer during January – June 1997*

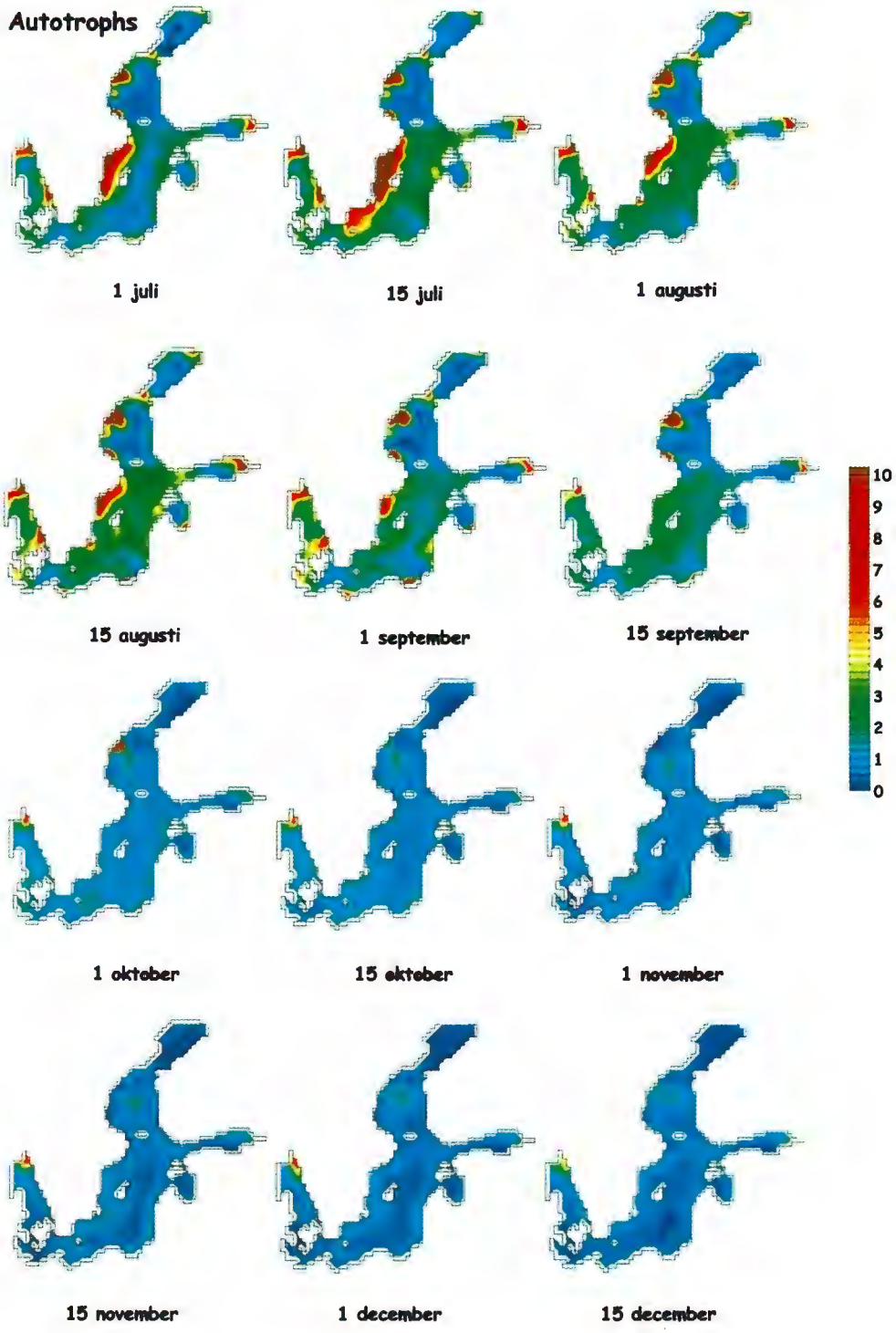


Figure 26 *Biweekly simulated autotroph concentration (µg chl l^{-1}) in the surface layer during July – December 1997*

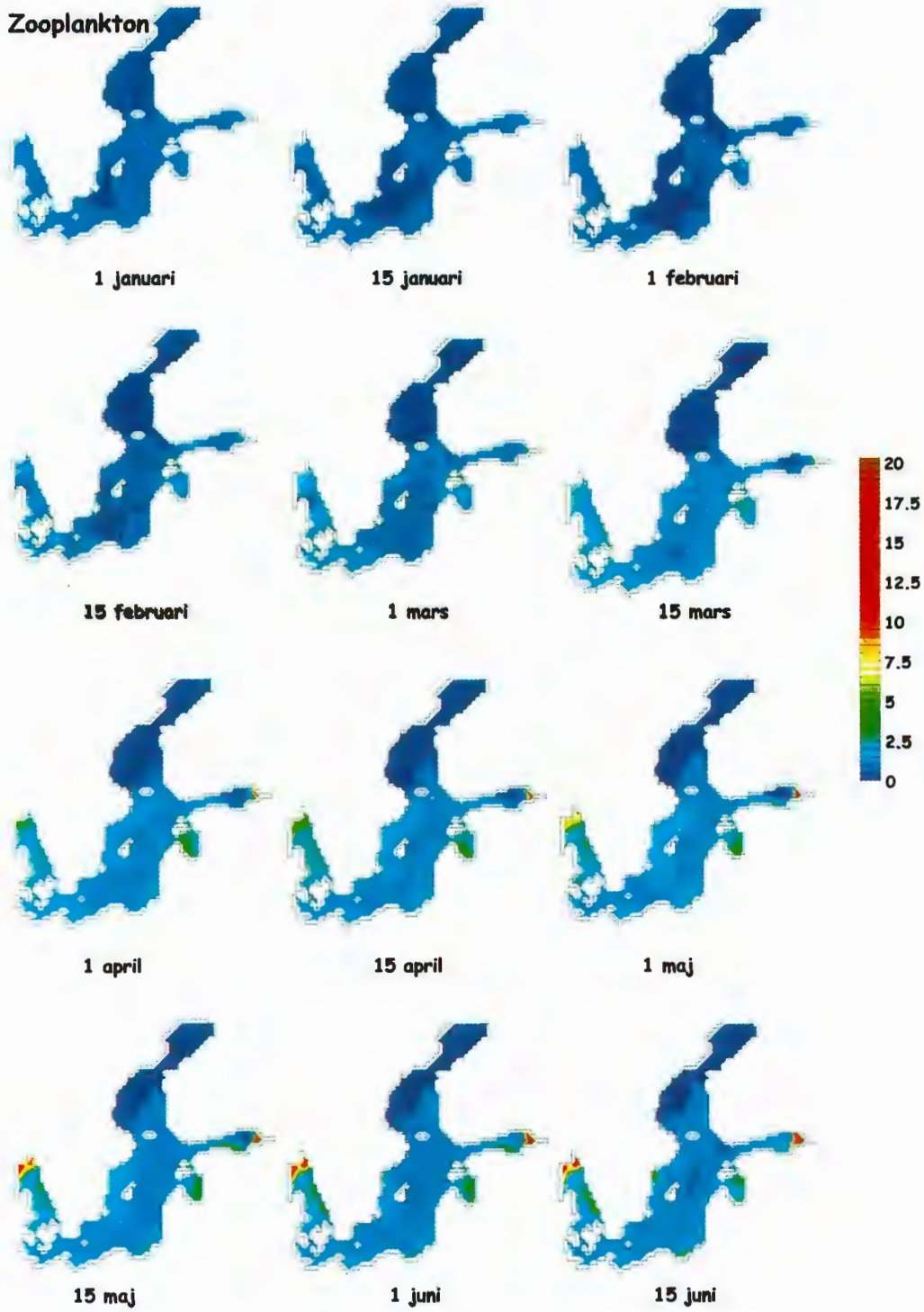


Figure 27 *Biweekly simulated zooplankton concentration (µg C l^{-1}) in the surface layer during January – June 1997*

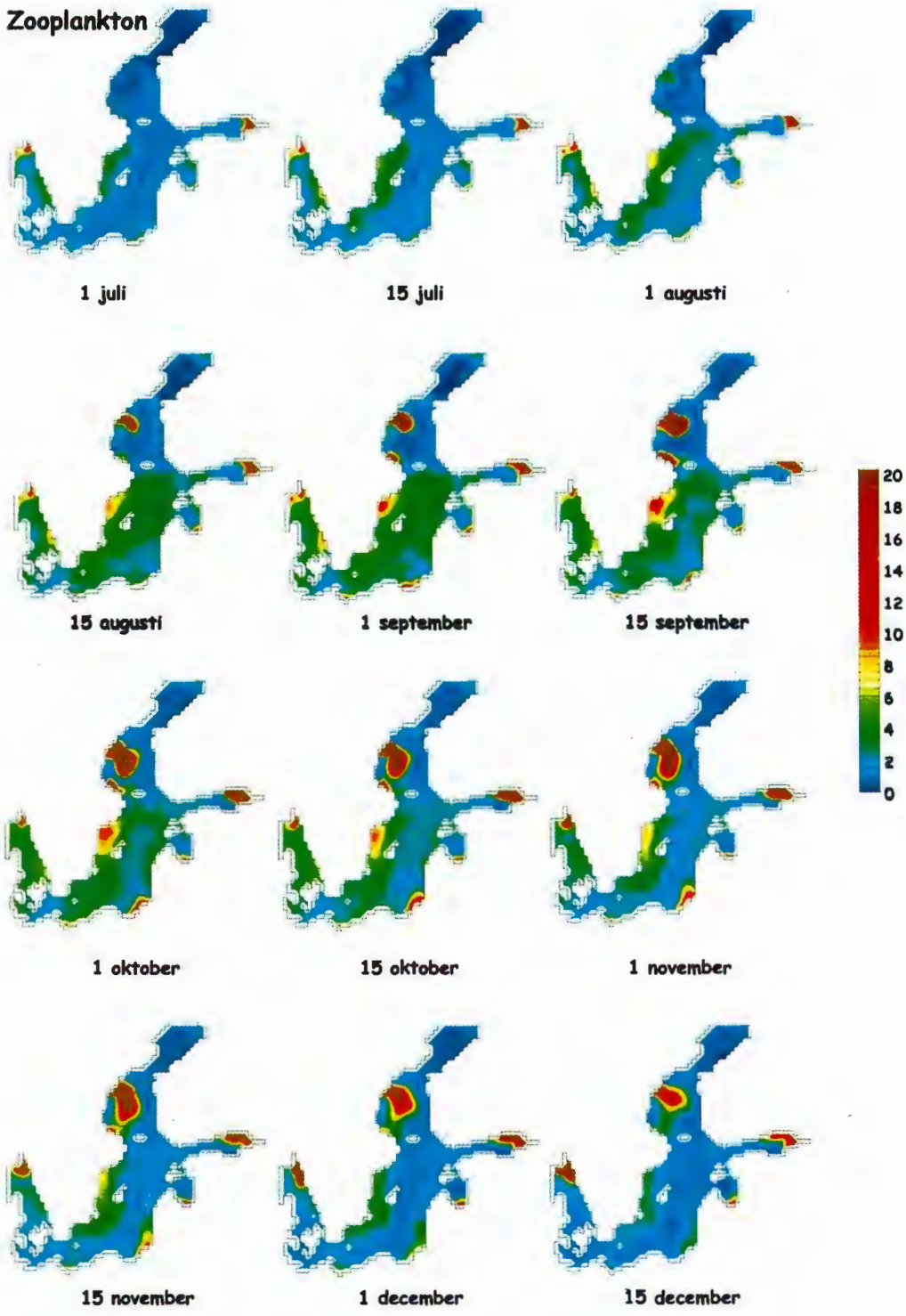


Figure 28 *Biweekly simulated zooplankton concentration (µg C l^{-1}) in the surface layer during July – December 1997*

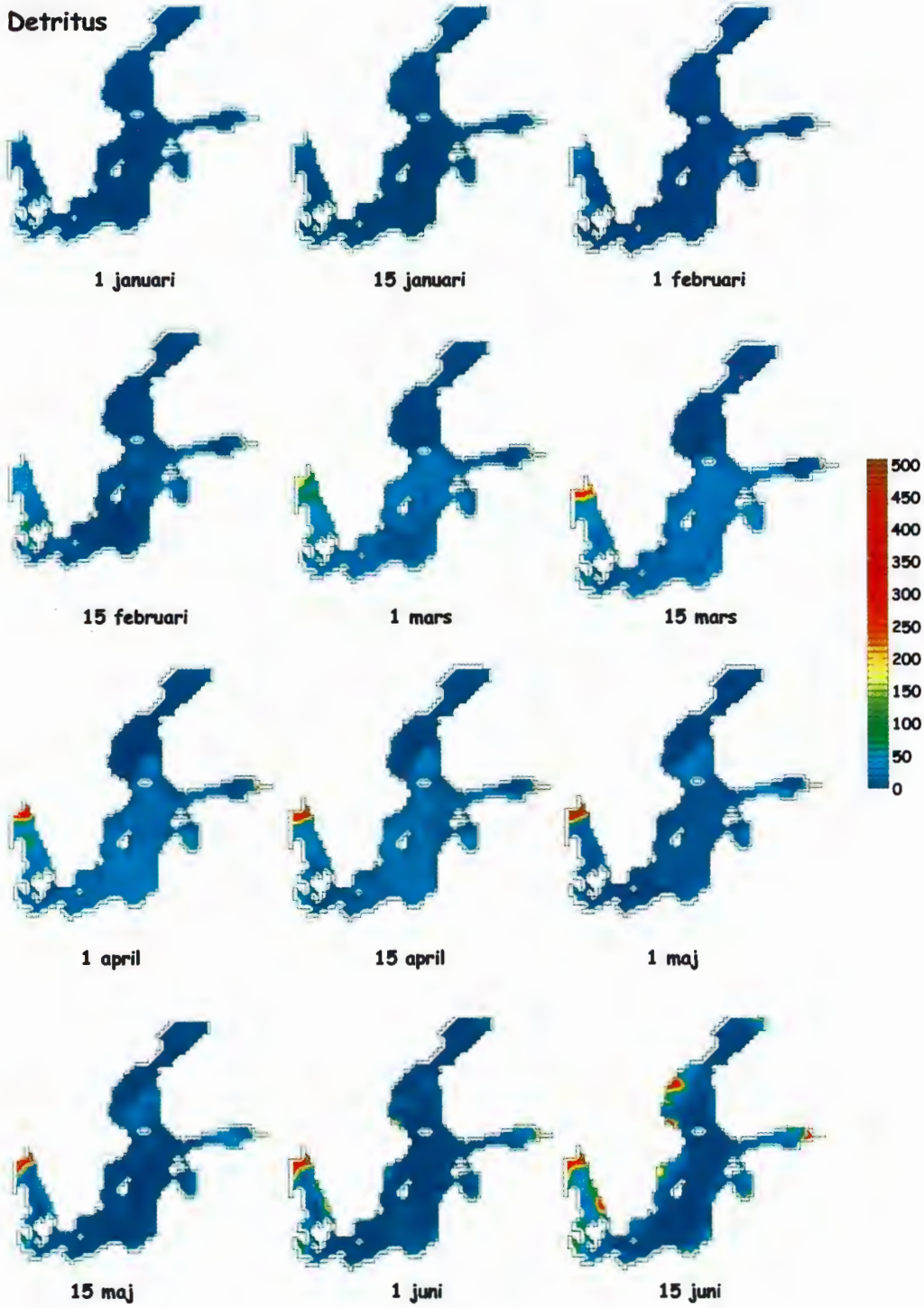


Figure 29 *Biweekly simulated detritus concentration (µg C l^{-1}) in the surface layer during January – June 1997*

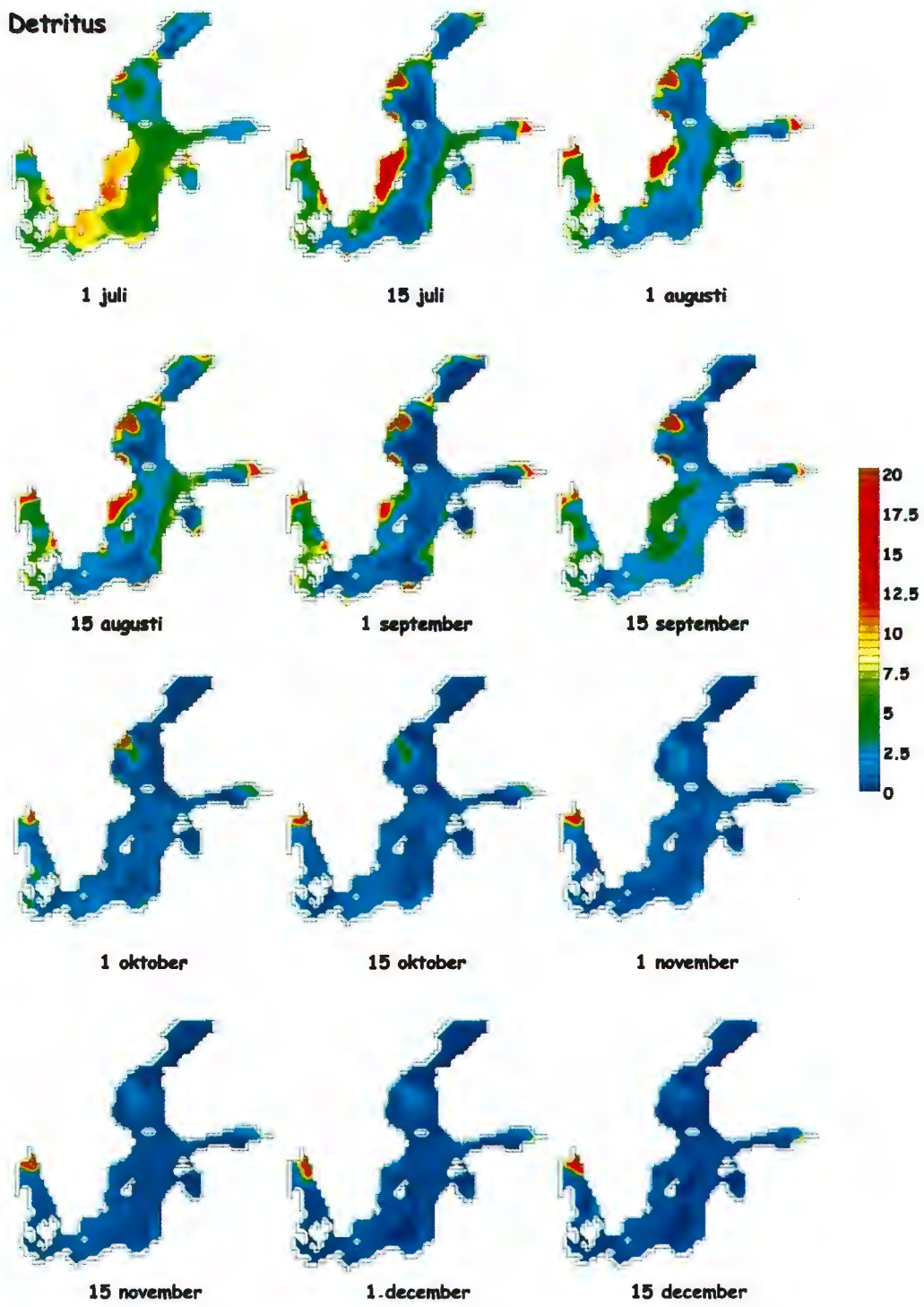


Figure 30 *Biweekly simulated detritus concentration (µg C l^{-1}) in the surface layer during July – December 1997*

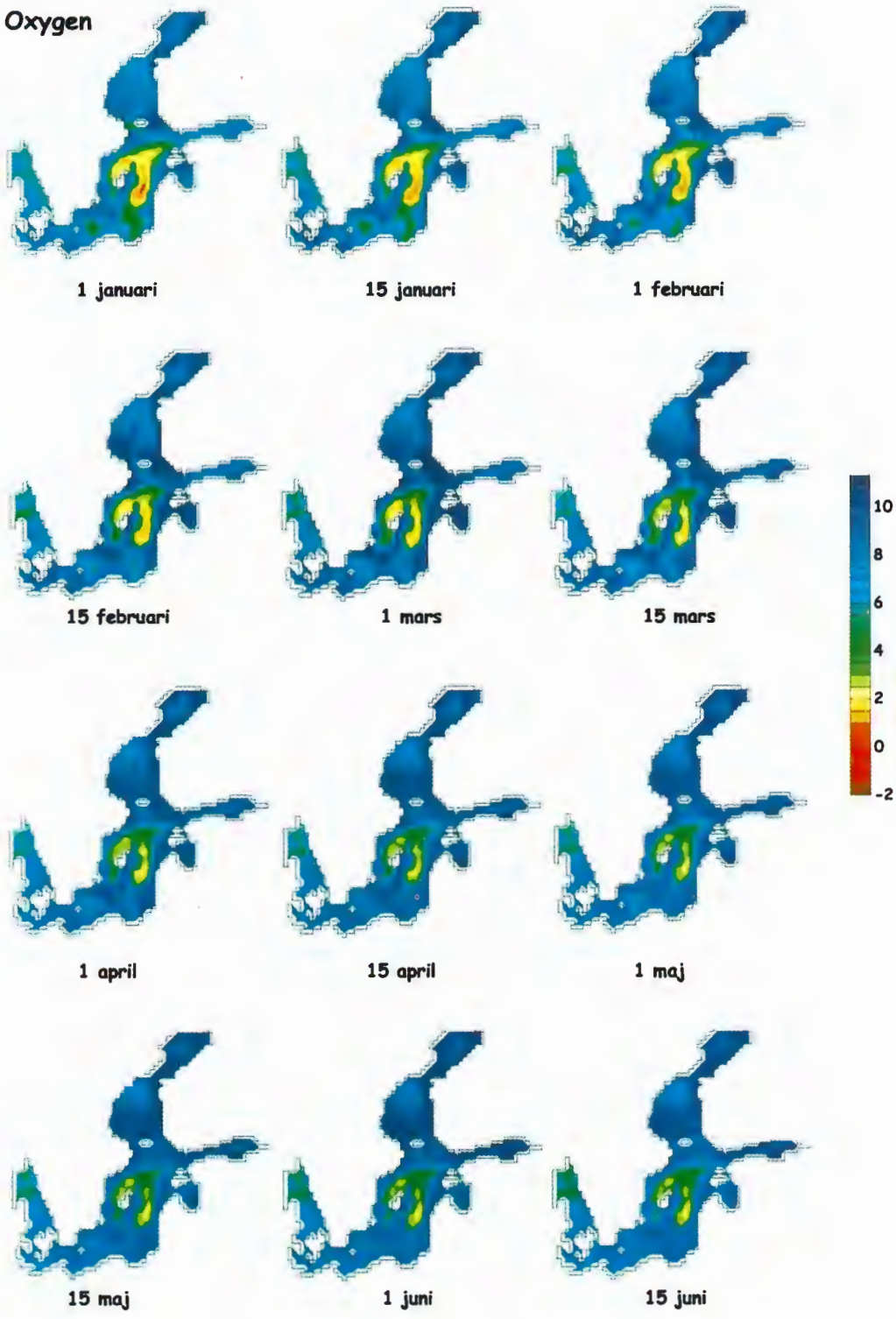


Figure 31 *Biweekly simulated oxygen concentrations.(ml l^{-1}) in the bottom layer during January – June 1997*

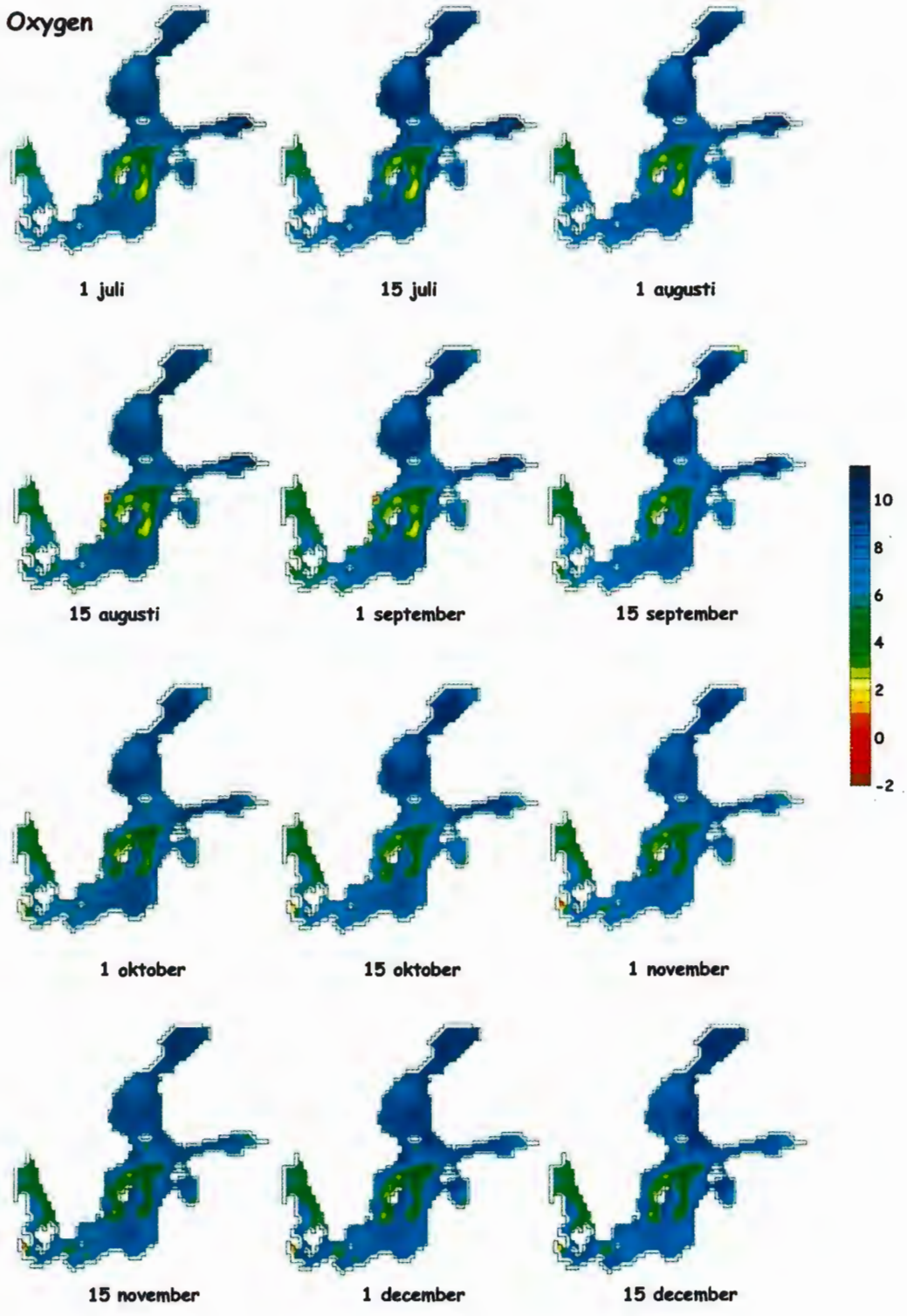


Figure 32 *Biweekly simulated oxygen concentrations.(ml l^{-1}) in the bottom layer during July – December 1997*

6.3 VALIDATION

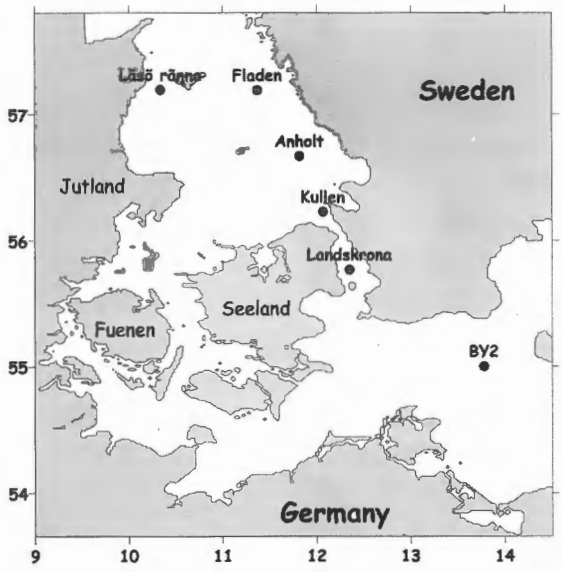


Figure 33 *The monitoring stations chosen for the validation. Note that the depth of the stations Läsö Ränna and Landskrona differs from the monitoring depths*

For the validation of the SCOBI 3D model we have focused on the Kattegat-Arkona area. The four stations, Fladen, Anholt, Kullen and BY2, Fig. 33, have been chosen for the validation as these are the most frequent visited monitoring stations in the area with water depth that best fit the model vertical resolution. Another two stations Läsö ränna and Landskrona have been added mostly for comparison with the model spring bloom dynamics. Both Läsö ränna and Landskrona monitoring stations are much deeper (40m) than the model vertical resolution (Läsö ränna 9m and Landskrona only 3m), Table 3.

Table 3 *Comparison of the maximum depths at the chosen validation stations. The coarse horizontal grid of the model causes the difference. The total depth at every grid point in the model represents an average depth of the 12× 12 nm area.*

Station	Maximum monitoring depth (m)	Maximium model depth (m)
Fladen	75	56
Anholt	55	25
Kullen	20	23
BY2	47	47
Landskrona	40	3
Läsö Ränna	40	9

Generally, the monitoring of ammonia is a bit tricky, especially in waters with high salinity. During 1997 the Swedish monitoring of ammonia still suffered from insufficient monitoring routines. Adding the fact that ammonia is known to be a nitrogen fraction with short lifetime in aerobic waters, it has been left out from the validation.

Vertically integrated monitored chlorophyll concentrations have been compared to vertically integrated modelled phytoplankton concentrations in order to study the models annual phytoplankton dynamics, Fig. 34. The vertical integration of the modelled phytoplankton concentration has been carried out from the surface to the bottom, whereas the monitoring of chlorophyll concentration has only been carried out down to 20 m depth. For the stations Fladen and BY2 this implies that the vertical integration of the model concentrations has been carried out for a depth of approximately twice or three times the monitored depth. Chlorophyll concentration has only been monitored once at the Kullen station during 1997. Chlorophyll from the Kullen station is therefore not included in the validation.

From the vertical integrated data from Kattegat stations Fladen and Anholt it is obvious that the SCOBI model has difficulties with catching the extreme early spring bloom in the Kattegat area Fig. 34. The modelled spring bloom culminates in late February, which agrees well with what is normal for the area. The reason for the early spring bloom has, to our knowledge not been properly explained, which complicates the adjustment of the model. One possible explanation can be that the weather was extremely calm and the water therefore was well stratified in combination with that the surface temperature was higher than normal. Normally, the spring bloom starts in a very thin layer of the order of one or a few meters. When the weather is calm this very thin layer survives for a long period and the plankton concentrations can reach high levels. With the vertical resolution of the model (4m in the surface layers) it is impossible to create such thin layers at the surface. The model probably exaggerates the mixing in the surface. The spin up of the model can be another explanation of the delay in the modelled Kattegat spring bloom.

The chlorophyll dynamics at the monitoring station Läsö Ränna differs from the other station after the spring bloom, when the chlorophyll concentration is held at a level, where the secondary bloom gradually reaches its maximum directly after the spring bloom ceases. The secondary bloom at the Läsö Ränna station is much less pronounced compared to the other stations. The same pattern can be seen from the modelled field. However, the secondary bloom ends earlier in the model than in reality.

At the Landskrona station, in the middle of the Sound, the secondary bloom is more intense than the spring bloom. In the model they are approximately of the same order, but at this station the model is only 3 m depth and the maximum concentration of autotrophs in the model is generally found at greater depths.

Entering the Baltic Proper (station BY2) the spring bloom in the SCOBI model occurs right in time or even a few days to early. However, the maximum spring bloom chlorophyll concentration is underestimated in the model. The secondary bloom in the late summer in BY2 occurs approximately one month earlier than data shows.

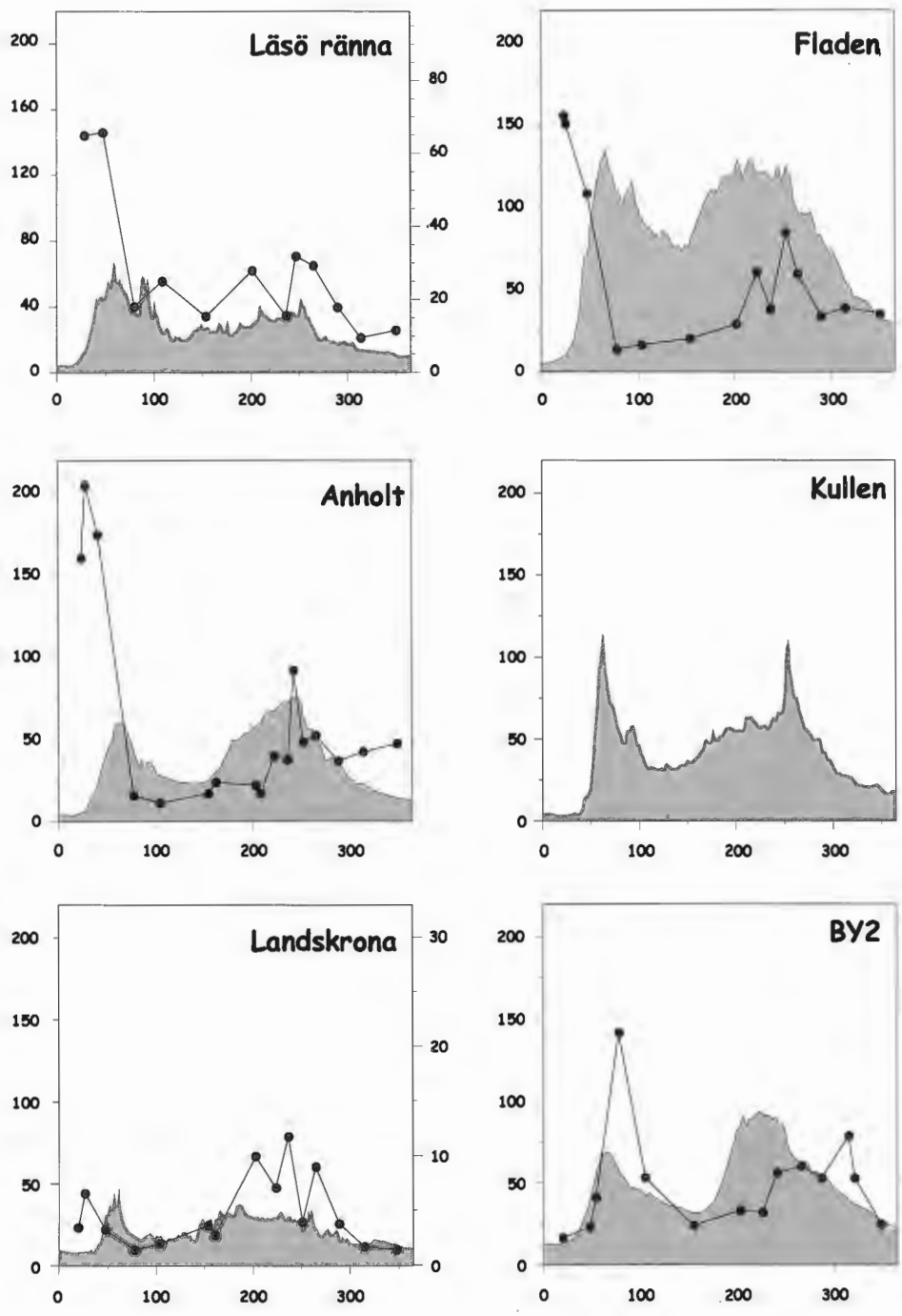


Figure 34 *Vertical integrated chlorophyll (mg chl m^{-2}) measurements for the upper 20 m (black line with dots) compared with vertical integrated autotroph concentration simulated by the SCOBI model (filled grey). The vertical integration of the model results has been carried out from the surface to the bottom. Chlorophyll is not measured at the Kullen station. For the stations Läsö ränna and Landskrona the model depth is much less than the total depth of the monitoring depth of chlorophyll. Duplicated y-axis has therefore been added to those panels where the right y-axis is associated to the model results. The integrated model results have been scaled with respect to the total depth at these locations.*

From scatter plots of salinity vs. nutrients, chlorophyll and oxygen from Fladen, Anholt, Kullen and BY2 one can see that a general problem is that the model underestimates the salinity in the deeper layers at all stations, Fig 35 and 36. At the northernmost station, Fladen, the salinity in the surface is overestimated in the model, (see also the vertically resolved timeseries in Fig. 37). It implies that the model stratification in the Kattegat is underestimated in the 12 nm grid resolution. A general impression when studying vertically resolved time series is that the model underestimates the nutrient concentrations in the deep water. But from the Figs. 35 and 36 one explanation can be that the water masses in the Kattegat is not properly described and that the water entering the Kattegat from the Skagerrak originates from shallower depths. In the salinity range of the model, maximum values of nutrients is underestimated in the Kattegat.

Undoubtedly, oxygen concentration is the variable that is best described by the model in the Kattegat. Generally the modelled oxygen concentrations follows the same pattern as the observations show, except for the highest salinities, where the lowest oxygen concentrations have been observed. From the vertically resolved timeseries, Figs. 37-39, it can be seen that low oxygen concentration is associated with high temperature as a result of increasing mineralisation both in the monitored field as well as the modelled field. However, the modelled temperature field differs slightly from the monitored temperature. The bottom temperature in autumn and winter is for example underestimated in the model. And consequently so is the local mineralisation and nitrification, which could explain the low deep-water nitrate concentrations in the model at the time.

The extreme chlorophyll concentration that was observed during the early spring bloom is not, as mentioned before, captured with the model. Besides that, the scatter plots in Figs. 35 and 36 show that the chlorophyll concentrations simulated by the model agree well with observations. From the vertically resolved time series at the station Anholt, Fig. 38, one conspicuous observation of high chlorophyll concentration in late summer is found at 10 m depth. This chlorophyll maximum rapidly established at the time, but had disappeared the following week. Rapid processes like that is not possible to catch with the model, instead the model has a chlorophyll maximum at the surface at the time.

Entering the Arkona Sea and the station BY2, model results, Fig. 36, differ from observation considerably. The model exaggerates oxygen concentrations in the deep layers. Phosphate and nitrate concentrations are consequently underestimated. The modelled hydrographical fields at BY2 differ considerably from the observations, both in salinity and temperature, Fig. 40. The high temperatures being observed near the bottom from late summer and through out the year is much more pronounced at BY2 than in the Kattegat and probably the explanation for the differences between the model and reality due to low mineralisation and nitrification rates.

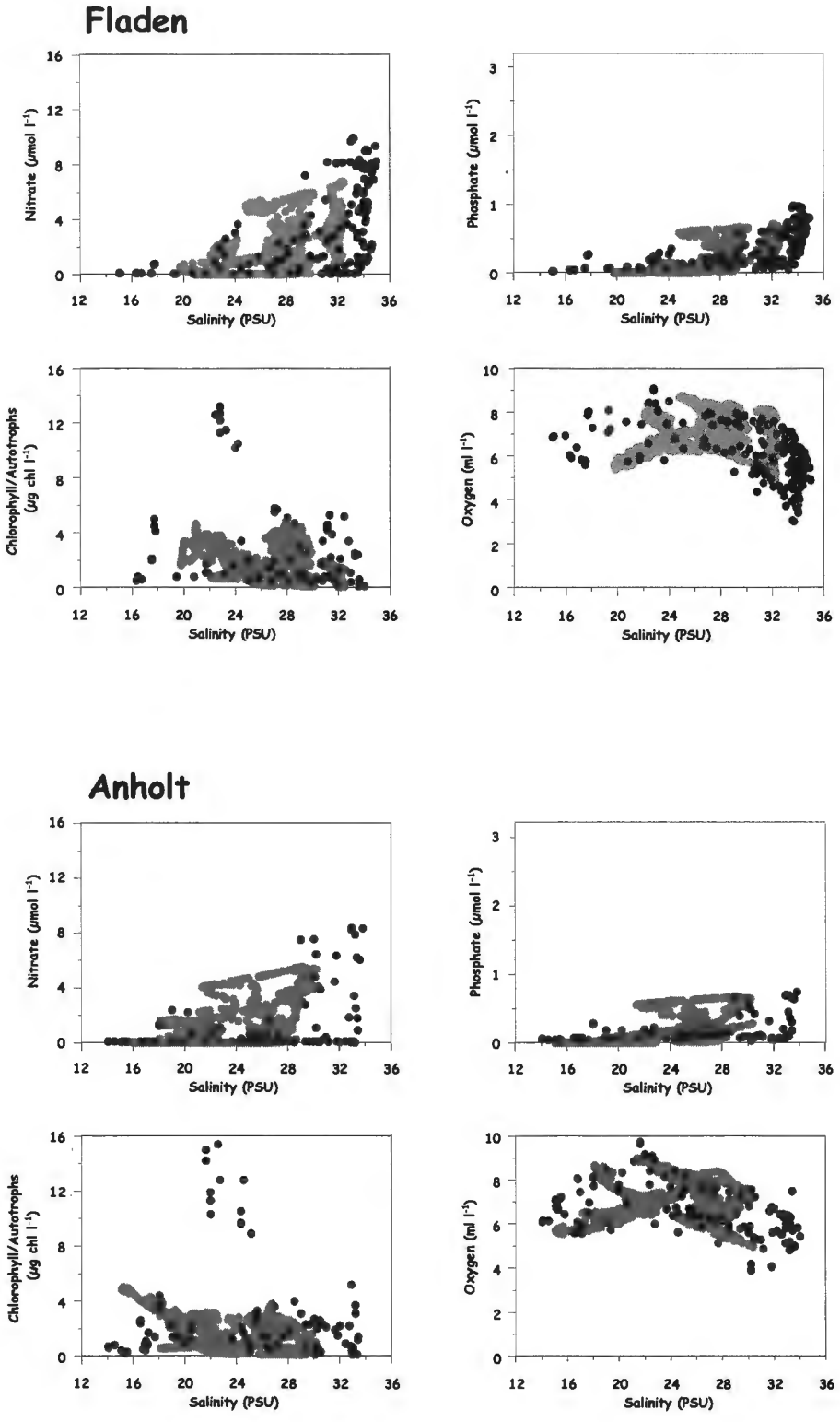


Figure 35 *Scatterplots for salinity vs nitrate, phosphate, chlorophyll/autotrophs and oxygen respectively. Black represents observations and grey modelled concentrations*

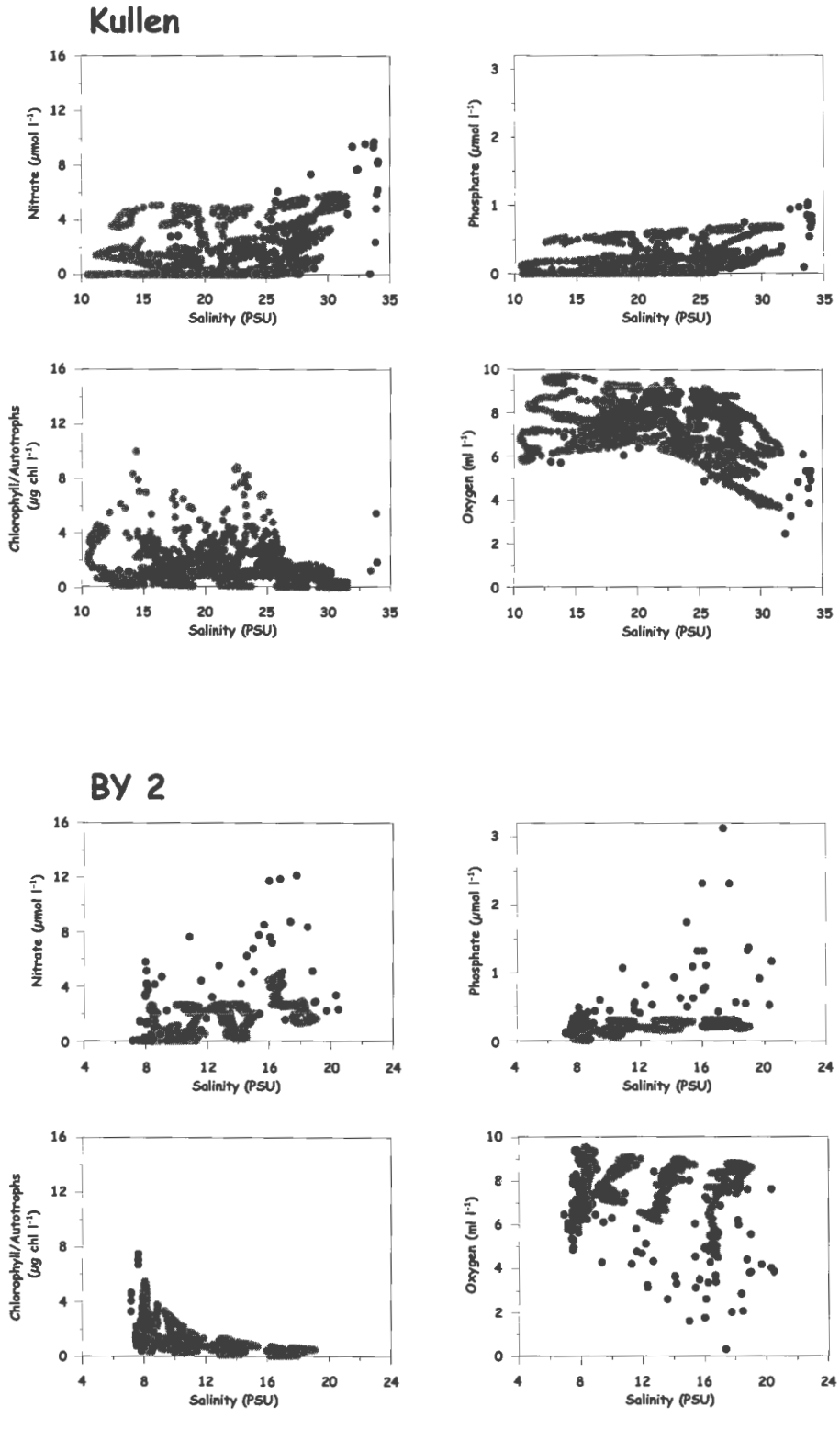


Figure 36 *Scatterplots for salinity vs nitrate, phosphate, chlorophyll/autotrophs and oxygen respectively. Black represents observations and grey modelled concentrations*

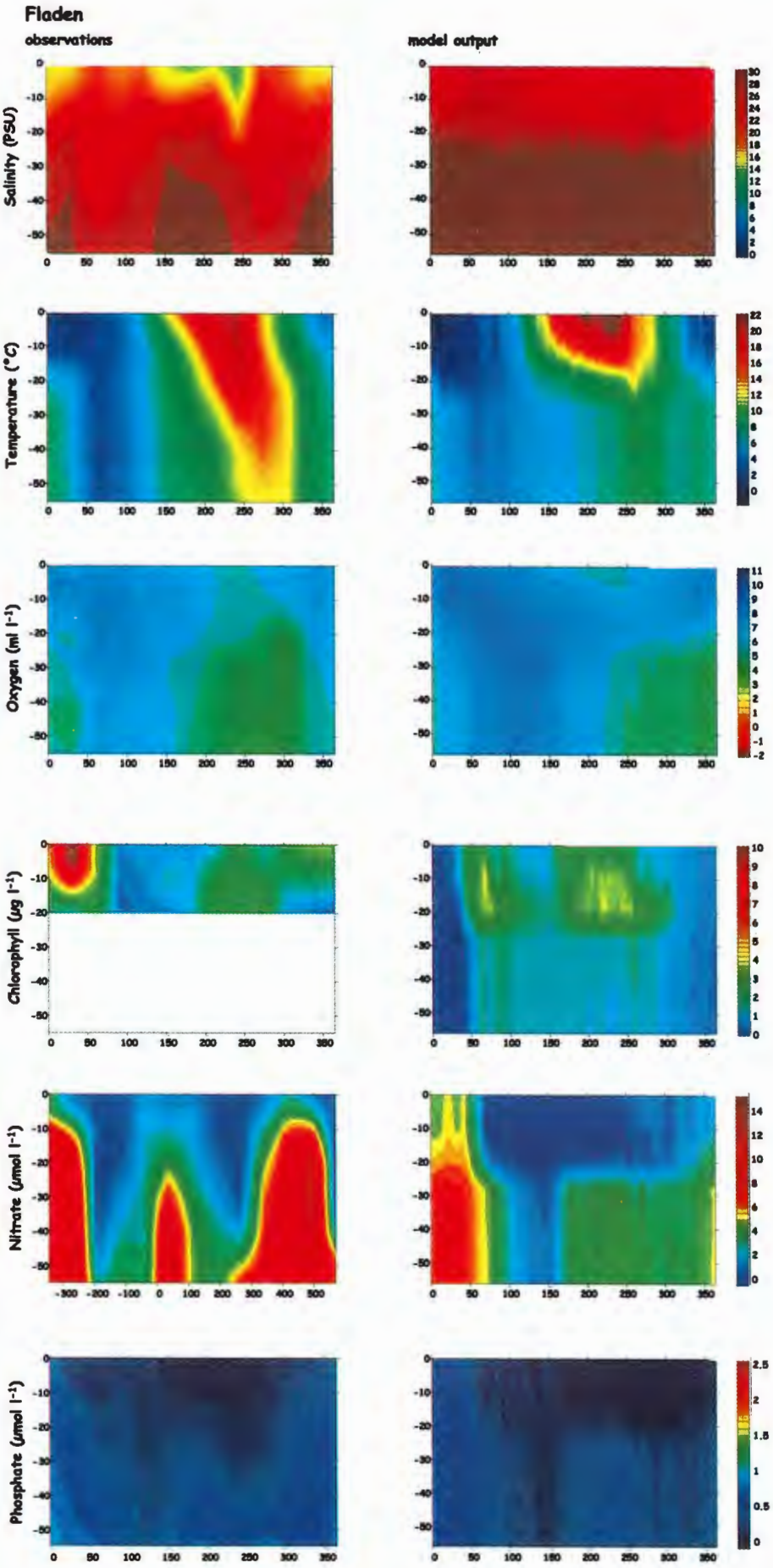


Figure 37 *Time series of observed and modelled fields from the Fladen station*

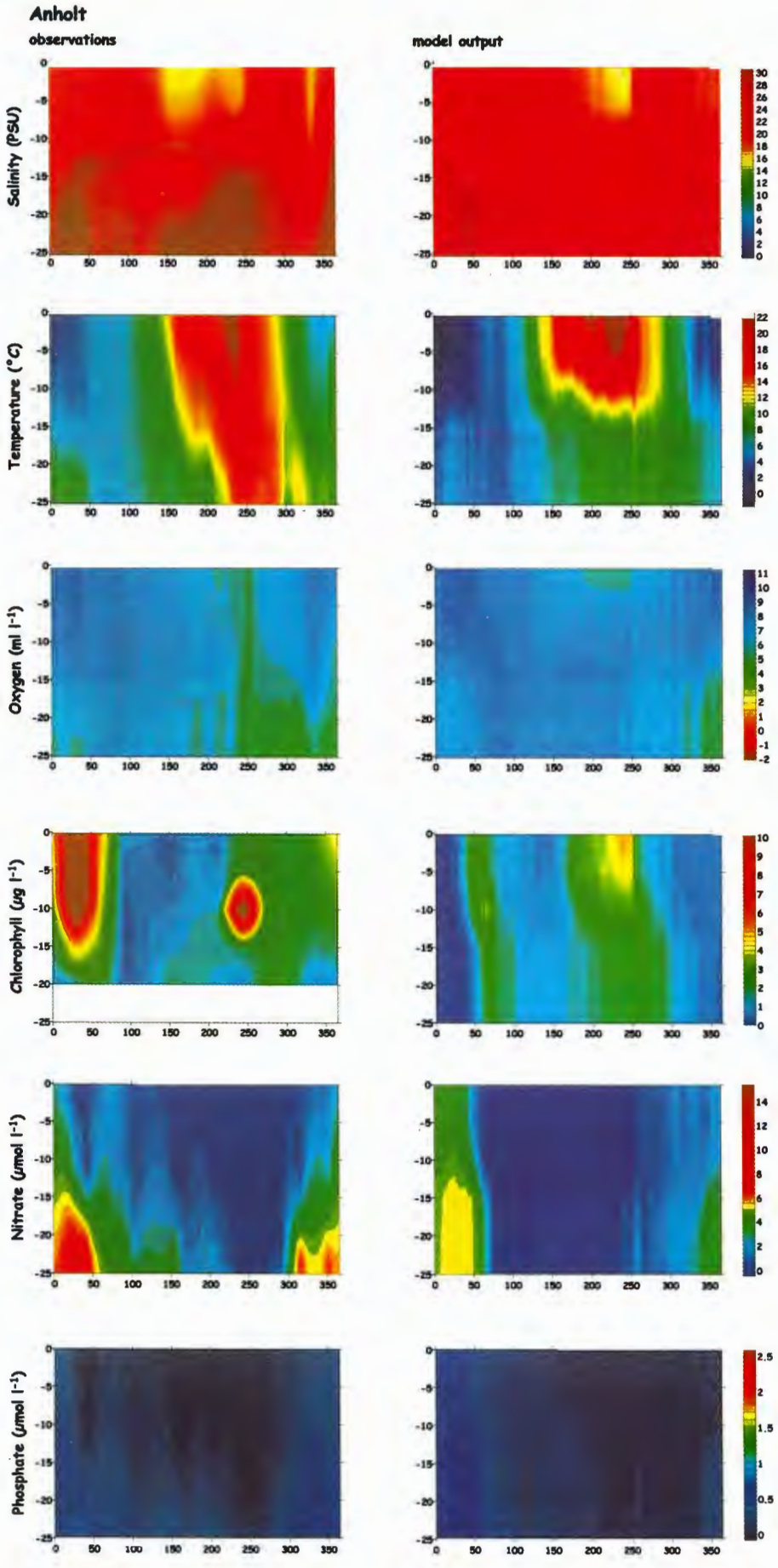


Figure 38 *Time series of observed and modelled fields from the Anholt station*

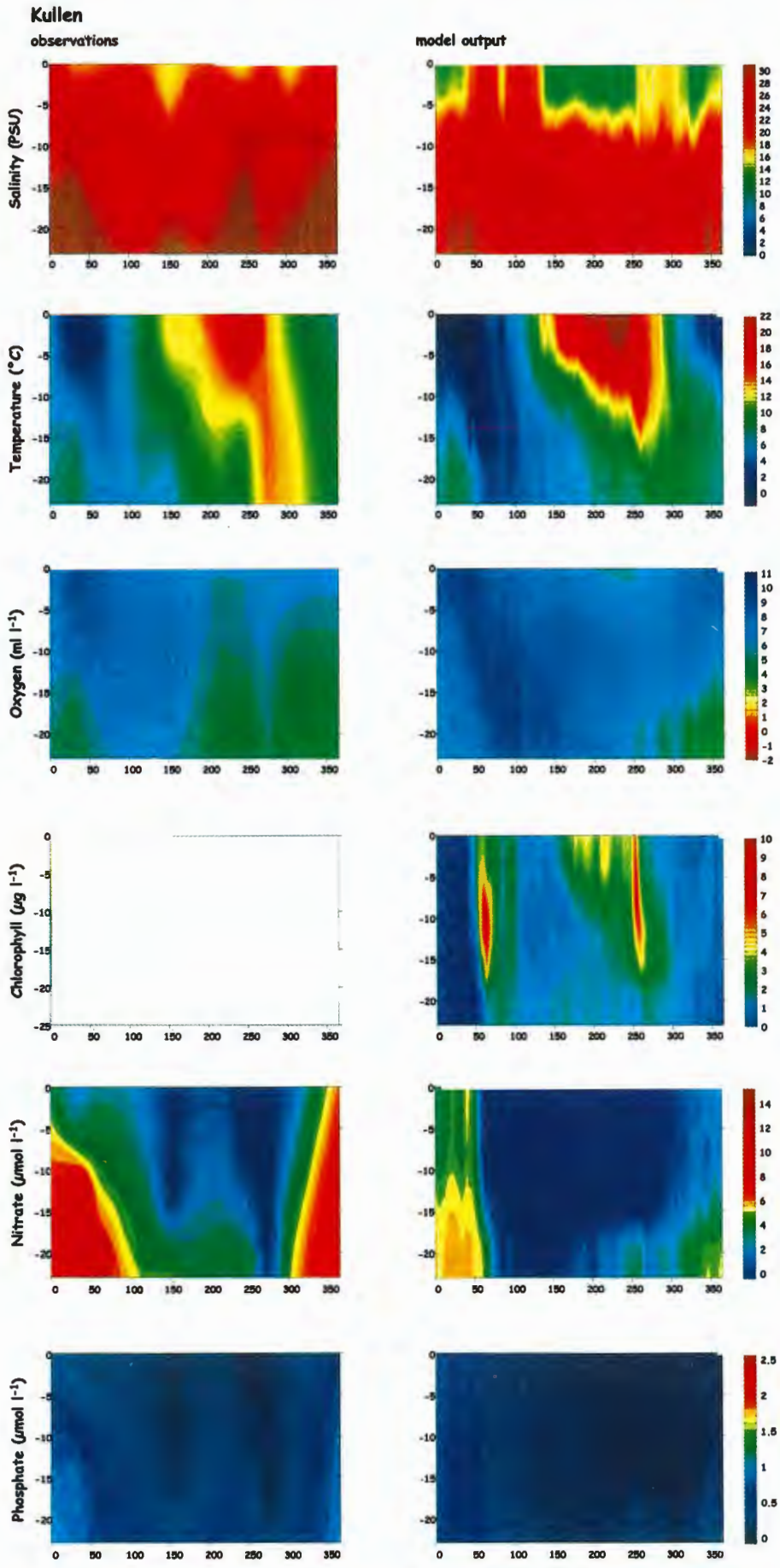


Figure 39 Time series of observed and modelled fields from the Kullen station

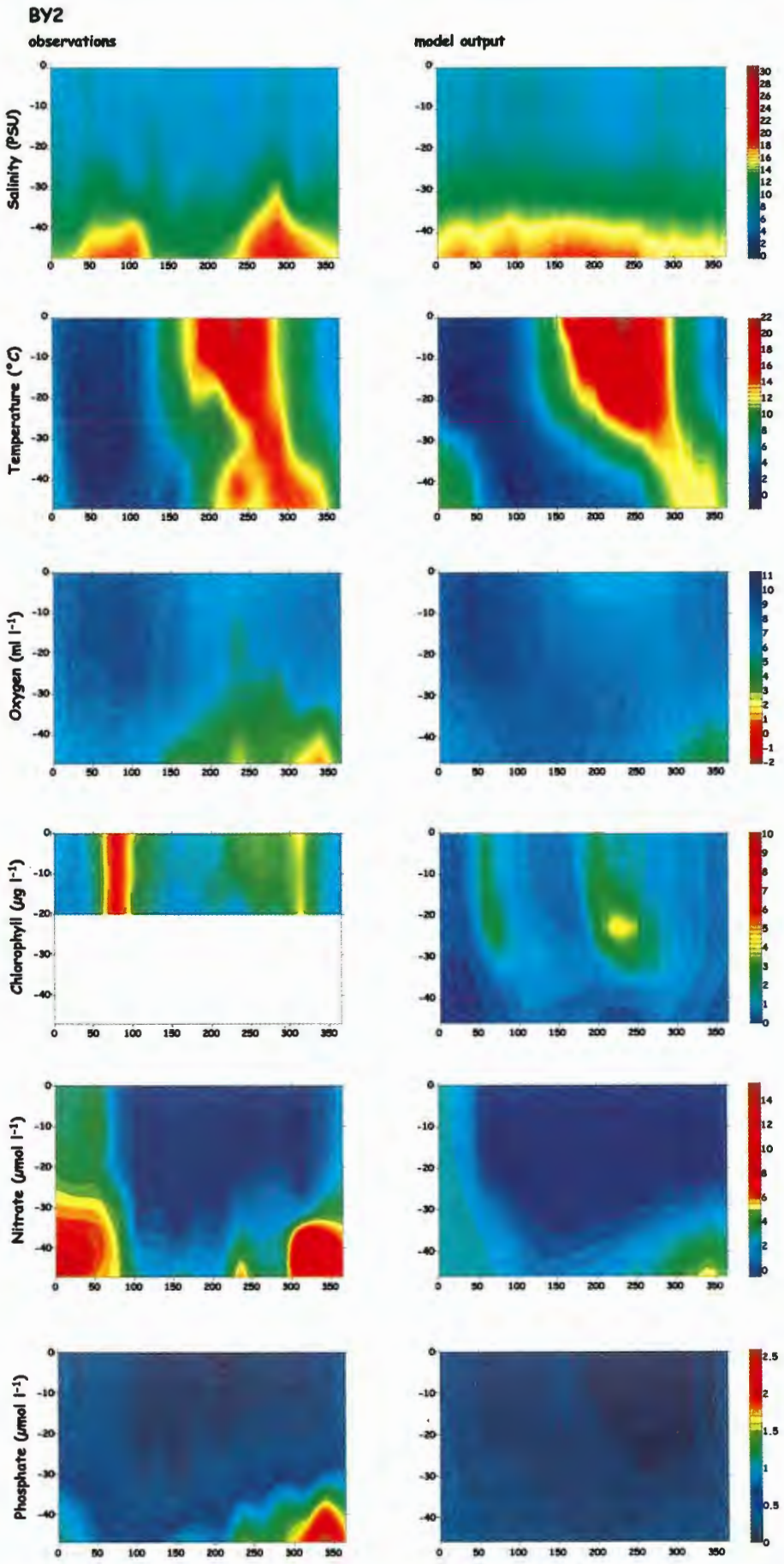


Figure 40 Time series of observed and modelled fields from the BY2 station

7 SUMMARY

The SCOBI model has been coupled to the 3D hydrographical model HIROMB for the Baltic Sea–Kattegat–Skagerrak area, with the emphasis on the development of a tool for environmental decision-makers. The application focus on the model approach to obtain an instrument for evaluating the input of nutrients on the physical and biogeochemical status of a water body, taking into account the most important/critical processes. The goal has been to be able to describe the nutrient sources and pathways as well as their bioavailability going from land to the coastal area and into the open sea.

This project concentrated on developing an model system that integrates the marine 3D model HIROMB-SCOBI with the riverine model HBV-N and the atmospheric and chemical model MATCH for the land load and atmospheric deposition respectively and to improve the sediment module in the SCOBI model. In the frame of this project we have developed a prototype of an integrated 3D biogeochemical model system.

This study has shown that the SCOBI model is able to describe the annual plankton, nutrient and oxygen dynamics with the present model set up. The seasonal biogeochemical evolution, with an earlier spring bloom in the Skagerrak and Kattegat area and a somewhat delayed spring bloom in the Baltic Proper and eventually a spring bloom that starts in the Gulf of Bothnia, is produced by the model. The model also produces high phosphorous concentrations west of the Gotland Island, which is typical for the area according to observations. In late summer, during the nitrogen fixating cyanobacteria bloom, the surface layer west of the Gotland Island is in the model completely emptied with phosphorous. As the nitrogen fixation ends the phosphorous concentration is regained. This annual cycle of phosphorous is known from observations. Accordingly, the model produces maximum autotroph concentrations during the secondary bloom between the Swedish mainland and the Gotland Island. This secondary bloom is mainly due to nitrogen fixation in the Baltic Proper. Nitrogen fixation is limited by phosphorous availability.

The formulation of the sedimentation of phytoplankton and detritus has been found to be crucial for the annual plankton dynamics in the area. It is a well-known fact that a chlorophyll maximum is found in the vicinity of the pycnocline during production season. To be able to create the chlorophyll maximum in the SCOBI model a reduction of the sinking velocity has been introduced with respect to the vertical stratification of the water mass. The formulation of the sinking reduction works well in well-stratified waters, but has to be calibrated further to become realistic in less stratified waters as in the Gulf of Bothnia.

The study has also shown how sensitive the biogeochemistry is to the hydrodynamics. To further improve the SCOBI 3D model it is necessary to extent the horizontal and vertical resolution in the circulation model. It would also be of great importance to further increase the vertical resolution in the

surface layer to get a better description of the often so explosively spring bloom development.

8 ACKNOWLEDGEMENT

The project has partly been financed by the Nordic Council of Ministers. Many of our colleagues at the SMHI have been involved with creating this integrated model system. We specially want to thank Dr. Maja Brandt and Mr. Jörgen Sahlberg supplying us with riverine data, Ms. Elisabeth Roos for the atmospheric deposition data and Mr. Michael Kolax for coupling the hydrological model fields and the meteorological model fields into SCOBI-3D. We also wish to thank Mr. Lennart Funkqvist and Dr. Andreas Eigenheer for the introduction to the HIROMB world.

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APPENDIX A

NOTATIONS OF THE VARIABLES IN THE SCOBI MODEL

Notation	Description	Unit
NO3	Nitrate	µmol N/l
NH4	Ammonia	µmol N/l
PO4	Phosphate	µmol P/l
A	Autotrophs	µg chl/l
Z	Zooplankton	µg C/l
D	Detritus	µg C/l
O2	Oxygen	ml/l
$\mathbf{B_N}$	Benthic inorganic nitrogen	µmol N/l
$\mathbf{B_P}$	Benthic inorganic phosphorous	µmol P/l

APPENDIX B

MATHEMATICAL FORMULATION OF THE BIOGEOCHEMICAL SINKS AND SOURCES IN THE SCOBI MODEL

Φ_Γ	Mathematical formulation	References
ASSIM	$\mu_{max} \cdot \min(\mu_{LIGHT}, \text{ASSIMP}, \text{ASSIMN} + \text{ASSIMA})$	
ASSIMA	$\frac{\mathbf{NH4}}{k_A + \mathbf{NH4}} \cdot \text{anox} \cdot \mathbf{A}$	DUGDALE (1967)
ASSIMN	$\frac{\mathbf{NO3}}{k_N + \mathbf{NO3}} \cdot e^{-\psi \cdot \mathbf{NH4}} \cdot \text{anox} \cdot \mathbf{A}$	DUGDALE (1967), WROBLEWSKI (1977)
ASSIMP	$\frac{\mathbf{PO4}}{k_P + \mathbf{PO4}} \cdot \text{anox} \cdot \mathbf{A}$	DUGDALE (1967)
DECOMP	$T_s \cdot \mathbf{D}$	SAVCHUK & WULFF (1996)
DECSINK	$c_{sink} \cdot ws_{det} \cdot \mathbf{D}$	
EXCPRED	$(1-\Omega) \cdot \text{PRED}$	FASHAM et al. (1990)
EXCR	*e-GRAZ*	FASHAM et al. (1990)
FAECAL	*f-GRAZ*	FASHAM et al. (1990)
FOT	$v_{tr} \cdot (\mathbf{O2} - O_2^S \cdot (1+\beta))$	STIGEBRANDT (1991)
GRAZ	*GRAZD+GRAZP*	FASHAM et al. (1990)
GRAZD	$\gamma\lambda_D \frac{\mathbf{D}^2}{k_f \cdot (\lambda_1 \mathbf{A} + \lambda_2 \mathbf{D}) + \lambda_1 \mathbf{A}^2 + \lambda_2 \mathbf{D}^2} \cdot \mathbf{Z}$	FASHAM et al. (1990)
GRAZA	$\gamma\lambda_A \frac{\mathbf{A}^2}{k_f \cdot (\lambda_1 \mathbf{A} + \lambda_2 \mathbf{D}) + \lambda_1 \mathbf{A}^2 + \lambda_2 \mathbf{D}^2} \cdot \mathbf{Z}$	FASHAM et al. (1990)
MORT	$c_{mort} \cdot \frac{\mathbf{A}}{2 + \mathbf{A}} \cdot \mathbf{A}$	FASHAM et al. (1990)
MORTPRED	$\Omega \cdot \text{PRED}$	FASHAM et al. (1990)
NITFIX	$r_{max}^{nf} \cdot s_{nf} \cdot \min\left(\mu_{LIGHT}, \frac{\mathbf{PO4}}{k_{fix} + \mathbf{PO4}}\right) \cdot \text{anox} \cdot \mathbf{A}$	SAVCHUK & WULFF (1996)
NITR	$\begin{cases} T_s^{nit} \cdot \frac{1}{1+0.1 \cdot I} \cdot \frac{\mathbf{O2}}{0.01+\mathbf{O2}} \cdot \mathbf{NH4} & \text{when } \mathbf{O2} > 0 \\ 0 & \text{otherwise} \end{cases}$	SAVCHUK & WULFF (1996)
PRED	$\xi \frac{\mathbf{Z}}{k_{Zoo} + \mathbf{Z}} \cdot \mathbf{Z}$	STEELE & HENDERSON (1992)
REG	$r \cdot \mathbf{B}$	STIGEBRANDT & WULFF (1987)

Φ_Γ	Mathematical formulation	References
REGA	$\begin{cases} 0 & \text{if } \mathbf{O_2} > 0.5 \\ r \cdot \mathbf{B} & \text{otherwise} \end{cases}$	STIGEBRANDT & WULFF (1987)
REGN	$\begin{cases} r \cdot (1-\Delta) \cdot \mathbf{B} & \text{if } \mathbf{O_2} > 0.5 \\ 0 & \text{otherwise} \end{cases}$	STIGEBRANDT & WULFF (1987)
REGP	$r \cdot (1-\infty) \cdot \mathbf{B}$	SAVCHUK & WULFF (1996)
SINK	$c_{sink} \cdot \min(0.2 \cdot \mathbf{A}^2, 3.0) \cdot \mathbf{A}$	STIGEBRANDT & WULFF (1987)
WDENIT	$\begin{cases} \alpha_{den} \cdot anox_d \dfrac{\mathbf{NO3}}{k_{den} + \mathbf{NO3}} \cdot \mathbf{NO3} & \text{if } \mathbf{NO3} > 0 \\ 0 & \text{otherwise} \end{cases}$	SAVCHUK & WULFF (1996)

APPENDIX C

FUNCTIONAL RESPONSES IN THE BIOGEOCHEMICAL SINKS AND SOURCES OF THE SCOBI MODEL

Functional responses		
anox	$\frac{1}{1+\left(\frac{o_{cr}^2}{\mathbf{O2}}\right)^{oxcr}}$	Reduction of anabolism during anoxic condition SAVCHUK & WULFF (1996)
μ_{max}	$0.8 \cdot e^{0.0633 \cdot T°C}$	Maximum phytoplankton growth due to temperature, EPPLEY (1972)
μ_{LIGHT}	$\frac{I}{I_{OPT}} \cdot e^{1-\frac{I}{I_{OPT}}}$	Maximum phytoplankton growth due to light,
I	$I_0 \cdot e^{-k \cdot z}$	Available light
λ_A	$\frac{\lambda_1 \mathbf{A}}{\lambda_1 \mathbf{A} + \lambda_2 \mathbf{D}}$	Relative supply of phtyoplankton
λ_D	$\frac{\lambda_2 \mathbf{D}}{\lambda_1 \mathbf{A} + \lambda_2 \mathbf{D}}$	Relative supply of detritus
$anox_d$	$\frac{1}{1+\left(\frac{\mathbf{O2}}{O_2^d}\right)^{cr_{den}}}$	SAVCHUK & WULFF (1996)
r_{nf}^{max}	$\frac{r_{nf}^{pm}}{1+e^{a_{nf}-b_{nf} \cdot T°C}}$	Maximum nitrogen fixation, SAVCHUK & WULFF (1996)
s_{nf}	$\frac{1}{1+\left(\frac{\mathbf{NO3}+\mathbf{NH4}}{\mathbf{PO4} \cdot npP}\right)^4}$	Nitrogen fixation capacity, SAVCHUK & WULFF (1996)
T_s	$a_{dec} \cdot e^{b_{dec} \cdot T°C}$	Mineralisation rate of detritus, SAVCHUK & WULFF (1996)
T_s^{nit}	$a_{nit} \cdot e^{b_{nitr} \cdot T°C}$	Nitrification rate, SAVCHUK & WULFF (1996)
R	$\varepsilon \cdot a_{reg} \cdot e^{b_{reg} \cdot T°C}$	Benthic mineralisation rate, STIGEBRANDT & WULFF (1987)
Δ	$\max\left(\frac{\mathbf{NO3}}{k_\Delta + \mathbf{NO3}}, 50\%\right)$	Benthic denitrification, STIGEBRANDT & WULFF (1987)
∞	$\frac{\omega_1 \cdot \mathbf{O2}}{\omega_2 + \mathbf{O2}}$	Benthic sequestred phosphate, SAVCHUK & WULFF (1996)

Functional responses		
v_{tr}	$5.9 \cdot \frac{a \cdot W + b}{\sqrt{Sc}}$	Transfer velocity through the sea surface, LISS & MERLIVAT (1986). W denotes the wind speed.
Sc	$1445 - 67.4 \cdot T°C + 0.91 \cdot (T°C)^2$	Analytical expression for the Schmidt number valid in the temperature range of 0 - 40 °C, MARMEFELT (2000)
O_2^s	$e^{\left[-173.4292 + \frac{249.6339 \cdot 100}{T°C} + 143.3483 \cdot \ln\left(\frac{T°C}{100}\right) \frac{21.8492}{100} \cdot T°C + \left(-0.033096 + \frac{0.014259}{100} \cdot T°C - \frac{0.0017}{10000} \cdot T°C^2\right) S\right]}$	Oxygen saturation concentration, WEISS (1970)

APPENDIX D

CONSTANTS USED IN THE SCOBI MODEL

Constant		comments
k_N	1.0	Halfsaturation constant for nitrate assimilation
k_A	1.0	Halfsaturation constant for ammonia assimilation
k_P	1.0	Halfsaturation constant for phosphate assimilation
c_{sink}	$\begin{cases} 1 \text{ when } \frac{\partial \rho}{\partial z} \le 0.01 \\ 1 - \frac{1}{0.2-0.01} \cdot \left(\frac{\partial \rho}{\partial z} - 0.01 \right) \text{ when } 0.01 < \frac{\partial \rho}{\partial z} < 0.2 \\ 0 \text{ when } \frac{\partial \rho}{\partial z} \ge 0.2 \end{cases}$	c_{sink} has been introduces in order to take into account plankton/detritus changes in relative buoyancy vs the sea water
Ws_{det}	1.5	Maximum detrital sinking velocity
c_{mort}	0.08	Maximum mortality rate per day
I_{OPT}	$\max(I_0, 25)$	Optimal light for phytoplankton growth, GARRADA et al. (1983), STIGEBRANDT & WULFF (1987); I_0 denotes the absorbed solar radiation at the sea surface.
k	$0.15 + 0.025 \cdot A_N$	Attenuation constant, KIRK (1983); A_N denotes the nitrogen content of the autotrophs according to the Redfield ratio.
γ	0.3	Maximum zooplankton grazing per day, FASHAM et al. (1990)
λ_1	0.75	Zooplankton preference for phytoplankton
λ_2	0.25	Zooplankton preference for detritus
k_f	50	Halfsaturation constant for zooplankton grazing.
α_{den}	0.5	Maximum denitrification per day, SAVCHUK & WULFF (1996)
O_2^d	0.504	Concentration at which the denitrification starts, SAVCHUK & WULFF (1996)
cr^{den}	6.0	SAVCHUK & WULFF (1996)

Constant			comments
k_{den}	1.0		Halfsaturation constant for denitrification, SAVCHUK & WULFF (1996)
Ω	0.3		Natural mortality rate of zooplankton predators, FASHAM et al. (1990)
r_{nf}^{pm}	0.5		Maximum nitrogen fixation rate, SAVCHUK & WULFF (1996)
a_{nf}	28.0		SAVCHUK & WULFF (1996)
b_{nf}	2.0		SAVCHUK & WULFF (1996)
npP	16		Redfield N/P ratio
k_{fix}	3.0		Halfsaturation constant for nitrogen fixation
e	0.3		Zooplankton excretion rate
a_{dec}	0.002		Maximum decomposition rate of detritus, SAVCHUK & WULFF (1996)
b_{dec}	0.15		SAVCHUK & WULFF (1996)
f	0.3		Zooplankton faecal production rate, FASHAM et al. (1990)
ξ	0.1		Maximum predation rate per day
k_{zoo}	1		Half-saturation constant for carnivorous grazing
ε	$\begin{cases}1\\0\end{cases}$	if $O2 < 0.5$ otherwise	STIGEBRANDT & WULFF (1987)
a_{reg}	0.0025		Maximum detrital mineralisation, STIGEBRANDT & WULFF (1987)
b_{reg}	0.15		STIGEBRANDT & WULFF (1987)
k_{Δ}	1.0		Half saturation contstant for benthic denitrification, STIGEBRANDT & WULFF (1987)
ω_1	7.5		SAVCHUK & WULFF (1996)

Constant		comments
ω_2	70.2	SAVCHUK & WULFF (1996)
a	$\begin{cases} 0.17 & W \le 3.6 \\ 2.85 \text{ for } & 3.6 < W \le 13 \\ 5.9 & W > 13 \end{cases}$	LISS & MERLIVAT (1986)
b	$\begin{cases} 0 & W \le 3.6 \\ -9.65 \text{ for } & 3.6 < W \le 13 \\ -49.3 & W > 13 \end{cases}$	LISS & MERLIVAT (1986)
β	0.025	Bubble factor, STIGEBRANDT (1991)
a_{nit}	0.01	Maximum nitrification rate. SAVCHUK & WULFF (1996)
b_{nit}	0.15	SAVCHUK & WULFF (1996)

APPENDIX E

SUBMODULE FOR SEDIMENT N AND P

THE MODEL SYSTEM

The Standard Eutrophication model has a simple description of sediment release of nitrogen and phosphorus. In this description a fraction of the nitrogen and phosphorus included in the settled organic matter to the sediment is returned back into the water column. This approach is proven sufficient when describing systems with moderate nutrient loading or with low retention time. However, in systems with high loading and/or high retention time the description is insufficient.

When modelling these systems the sediment module should be used.

The sediment module is an add-on module to the standard MIKE 3 EU model and therefore uses the state variables and some of the standard processes as input. Also, the sediment module is constructed in a way that makes it possible to use it in connection with other add on modules like the eelgrass module.

In figure 1 the state variables and processes of the standard EU module are presented. The sediment module and the EU module are inter linked through the sedimentation of organic material, including nutrients from the water column to the sediment and the exchange of inorganic nutrients between the sediment and water column.

The present description is restricted to the sediment but may use terms from the standard EU description.

N AND P CYCLE IN THE SEDIMENT MODULE

The state variables and the processes in the sediment module are listed below and presented in figures 2 and 3 for nitrogen and phosphorus, respectively.

State variable	Notation
Organic N in the sediment	**SON**
Total NH4	**SNH**
NO3	**SNO3**
Immobile nitrogen	**SNIM**
Leachable organic P	**SOP**
PO4-P in pore water	**SIP**
PO4-P adsorbed to Fe+++	**SPFE**
Immobile P	**SIMP**

The state variables, describing nitrogen in the sediment, are linked to plankton N, detritus N and inorganic N in the water by sedimentation of organic N or flux of NH4 and NO3 across the sediment surface. The organic N in the sediment is mineralised producing NH4, which enters the SNH pool. NH4 in the sediment may either be exchanged with inorganic N (IN) in the water or nitrified to NO3 in the uppermost layer of the sediment utilising O2.

The NO3 entering the SNO3 pool may either be denitrified or exchanged with inorganic N in the water. The nitrogen cycle in the sediment is described in figure 2.

A fraction of the plankton P and detritus P which settles on the sediment surface undergoes decomposition or is eaten by deposit feeders in the sediment before it is incorporated into the sediment. Some of the settled P will therefore be turned into PO4 immediately, while the rest enters the pool of organic P in the sediment. The FSPB and RSOP processes describe these fluxes of P, see fig. 3.

A fraction of the P entering the sediment surface will be buried in deeper sediment layers as chemically bound to apatite (CaCO3) or to refractory organic matter, JENSEN et al. (1995), SUNDBY et al. (1992). This is described in the model by letting a fraction of the organic P enter the pool of immobilised P (SIMP).

The pool of leachable organic P (SOP) is degraded to PO4 and released into the pore water pool of PO4 (SIP). Besides the organic P, the pool of adsorbed PO4 to oxidised Fe has shown to be the most important P component for the P cycle in marine coastal sediments. MORTENSEN (1992), JENSEN et al. (1995). Therefore a pool of PO4 adsorbed to Fe+++ has been included in the module (SPFE). Adsorption and desorption to Fe+++ is determined by the concentration of PO4 in the sediment.

Fe will only be on oxidised form in the layers with O2 or NO3. The thickness of these layers, is subject to changes over the year, and so will the pool of Fe+++ in the sediment. The Pool of Fe+++ , and thereby also the pool of SPFE, is made dependent on the penetration depth for NO3 in the sediment. Finally, a flux of PO4 across the sediment surface is included in the model as a function of the concentration difference between the water and the sediment PO4.

NITROGEN PROCESSES

The processes in a dynamic model describe the changes in concentrations and fluxes between state variables, i.e. nitrification of NH4 to NO3 in the sediment. Together with the state variables the processes may be regarded as the cornerstones in a dynamic model.

In the following, the processes involved in the nitrogen cycle are described in connection to the state variables.

ORGANIC N IN THE SEDIMENT (SON):

Input of new organic N to the sediment is mediated by sedimentation of living algae or dead organic mater from the overlaying water column. When the organic matter reaches the sediment surface, it often forms a loos layer of material, which is easily resuspended. Degradation of material, in this thin layer is fast compared to the under laying sediment. In the sediment, the organic material will degrade releasing nitrogen as NH4 to the pore water. However, as the C:N ration in the remaining organic matter increases the degradation decreases because the organic matter does not fulfil the needs of nitrogen for bacteria and other organisms involved in this mineralisation. At a molar C:N ratio of about 11 the net mineralisation of NH4 seems to stop BLACKBURN and HENRIKSEN (1983).

In the model the input of organic N to the sediment is calculated by the standard EU as sedimentation of algae N and detritus N, SEPN and SEDN respectively. A fraction of the settled organic N is assumed to be degraded immediately and returned to the pool of inorganic N in the water. This process (FSNB) is temperature dependent and should account for the relative fast mineralisation of organic material in the uppermost part of the sediment. The remaining organic N (RSON) is added to the pool of organic N in the sediment (SON).

A fraction of the settled nitrogen is assumed to be buried in the sediment. This fraction (RSNIM) is defined as the part of the settled nitrogen from the settled organic matter with a

C:N ratio above about 11. The pool of organic N is mineralised with NH4 as the end product, this process (RSONNH) is set at a temperature dependent fraction of SON

Mineralization of newly settled organic N:

$$FSNB = KRESN0 \cdot (SEDN + SEPN + SEEN) \cdot TETN^{(TEMP-20)} \quad (g\ N/m^3/d)$$

Input of N to the sediment pool of organic N:

$$RSON = (SEPN + SEDN + SEEN - FSNB) \cdot MADE \quad (g\ N/m^2/d)$$

Burial of organic N in the sediment:

if
$(SEPC + SEDC + SEEC) \cdot MADE \cdot KNIM \leq RSON$
then
$RSINM = (SEPC + SEDC + SEEC) \cdot MADE \cdot KNIM$ $(g\ N/m^2/d)$
else
$RSINM = RSON$

Mineralization of SON in the sediment:

$$RSONNH = SON \cdot KRSN1 \cdot TETN^{(TEMP-20)} \quad (g\ N/m^2/d)$$

TOTAL NH4 IN THE SEDIMENT (SNH):

The total NH4 in the sediment is defined as the NH4, which may be extracted with a KCl solution. A part, and sometime a major part, of this NH4 is loosely sorbed to particles in the sediment. In the model, it is assumed that the fraction is variable for nitrification and flux across the sediment surface. Three processes are connected to these state variables, mineralization of SON, nitrification, and flux of NH4 across the sediment- water surface. For mineralization of SON see the description of SON.

Nitrification is mediated by bacteria in the sediment by oxidising NH4 to NO2 and NO3 using O2. In the model nitrification is calculated by multiplying a potential nitrification capacity with a Monod kinetic for NH4 in the sediment and a Monod kinetic for squared O2 concentration in the water. As nitrification is an aerobic process, it will be restricted to the sediment layer where O2 is present.

The flux of NH4 between the sediment and the water is a process which is dependent of the concentration difference between the water and the sediment and the total diffusion for NH4.

In the standard EU model, NH4 and NO3 is lumped together as inorganic N (IN). It is therefore necessary to assume that the ratio of NH4 and NO3 in the water just above the sediment surface has the same ratio as in the sediment. First the flux of NH4 and NO3 across the sediment is calculated, and then the flux of NH4 is calculated.

Nitrification of total NH4 in the sediment

$$RSNIT = KNIT \cdot KDO2 \cdot \frac{SNH}{SNH + KSNH0} \cdot \frac{DO^2}{DO^2 + MDO} \cdot TETN^{(TEMP-20)} \quad (g\ N/m^2/d)$$

Flux of SNH + SNO3 between the sediment and the water

$$FNHNO3 = DIFN \cdot \frac{SNH + SNO3 - IN}{KDOX} \qquad (g\ N/m^2/d)$$

Flux of SNH between the sediment and the water

$$FNH = FNHNO3 \cdot \frac{SNH}{SNH + SNO3} \qquad (g\ N/m^2/d)$$

To be able to calculate the nitrification and the flux of SNH it is necessary to know the O2 and NO3 penetration into the sediment.

In coastal areas the O2 penetration in the sediment will be a few mm. An empirical relation has been established for a silty coastal sediment in Denmark, GUNDRESEN et al. (1995). This relation has been used in the model.

O2 penetration into sediment:

$$KDO2 = KKA + KKB \cdot DO - KKC \cdot ODSC \cdot MADE \qquad (m)$$

Below the oxygen layer NO3 will take over as an electron acceptor keeping Fe and Mn in oxidised form. The NO3 respiration or denitrification is mediated by bacteria in the sediment.

The penetration of NO3 can be calculated using Fikcs 1. low and assuming a constant denitrification, diffusion of NO3 with depth, knowing the NO3 concentration in the layer with O2 and assuming that the NO3 concentration is 0 at the depth KDOX.

NO3 penetration into the sediment is then:

Using Ficks 1st law and assuming steady state conditions:

$$0 = DIFN \cdot \frac{d^2C}{dx^2} + DNM3$$

By integration:

$$\frac{dC}{dx} = \frac{DNM3}{DIFN} \cdot x + a$$

The constant a can be defined using $\frac{dC}{dx} = 0$ for x = Kd

$$a = -\frac{DNM3}{DIFN} \cdot Kd$$

By yet another integration the concentration C can be found:

$$C = \frac{DNM3}{2 \cdot DIFN} \cdot x^2 - \frac{DNM3}{DIFN} \cdot Kd \cdot x + b$$

The constant b can be defined using C = 0 for x = Kd.

$$b = \frac{DNM3}{2 \cdot DIFN} \cdot Kd^2$$

$$KDOX = \sqrt{\frac{SNO3 \cdot 2 \cdot DIFN}{DNM3}} + KDO2 \qquad (m)$$

NO3 IN SEDIMENT (SNO3):

Three processes are determining the NO3 concentration in the sediment: nitrification, denitrification and flux of NO3 between the sediment and the water. The nitrification has been described under SNH.

The flux of NO3 across the sediment surface is calculated in the same way as the flux of NH4.

Flux of NO3 across sediment surface:

$$FNO3 = FNHNO3 - FNH \qquad (g\ N/m^2/d)$$

The denitrification (RDENIT) or flux of NO3 into the sediment is calculated using Ficks 1. Law.

DENITRIFICATION

$$RDENIT = -DIFN \cdot \frac{dC}{dx} \qquad \text{for } x = 0$$

For $\frac{dC}{dx}$ see under NO3 penetration into sediment

$$RDENIT = \sqrt{2 \cdot DIFN \cdot DNM3}$$

where

$$DNM3 = DEMAX \cdot TETN^{(TEMP-20)} \qquad (g\ N/m^2/d)$$

IMMOBILISATION OF N IN SEDIMENT (SNIM):

Immobilisation of N may occur either as burial of slowly degradable organic N or as denitrification of NO3. The processes have been described under SON and SNO3, respectively.

PHOSPHORUS PROCESSES

The below description of the phosphorus processes is made according to the state variables in the P cycle.

LEACHABLE ORGANIC P IN THE SEDIMENT (SOP):

SOP is a pool of leachable organic P, which is able to be transformed into PO4 by mineralization. Input to SOP occurs through sedimentation of algae P and detritus P to the sediment surface. A fraction of the settled organic P is mineralized on the sediment surface represented by the flux FSPB. However, a part of the settled P will be immobilised in the sediment either as refractive organic P or as appatite P. In the model the immobilisation is calculated as a fraction of RSOP which enters the pool of immobilised P, SIMP. The remaining of the total settled organic P enters the pool of SOP

Mineralization of newly settled organic P:

$$FSPB = KRESP0 \cdot (SEDP + SEPP + SEEP) \cdot TRSP^{(TEMP-20)} \qquad (g\ P/m^3/d)$$

Input of P to the sediment pool of organic P:

$$RSOP = (SEPP + SEDP + SEEP - FSPB) \cdot MADE \qquad (g\ P/m^2/d)$$

Burial of organic P in the sediment:

$$RSPIM = RSOP \cdot KPIM \qquad (g\ P/m^2/d)$$

Mineralisation of SOP in the sediment:

$$ROPSIP = SOP \cdot KRSP1 \cdot TRSP^{(TEMP-20)} \qquad (g\ P/m^2/d)$$

PO4 IN THE PORE WATER (SIP) AND PO4 ADSORBED TO FE+++ (SPFE):

PO4 in the pore water may either be adsorbed to Fe+++ (SPFE) or exchanged with inorganic P (PO4) in the water across the sediment surface. The equilibrium of PO4 adsorbed to Fe+++ is described as a product between a P sorption capacity, which is dependent of the amount of F+++, and a Monod relation of SIP, Jacobsen (1977) and (1978).

The adsorption or desorption of PO4 is then defined as the change in SPFE caused by a change in the concentration of SIP or a change in the amount of Fe+++, which is dependent of the penetration depth of NO3. (KDOX).

SORPTION AND DESORPTION OF PO4 TO FE+++

$$RFESIP = KRAP \cdot \left(KFE \cdot KFEPO \cdot \frac{SIP}{SIP + KHFE} \cdot VF \cdot DM \cdot 10^6 \cdot KDOX - SPFE_{t-1} \right) \qquad (g\ P/m^2/d)$$

FLUX OF PO4 BETWEEN THE SEDIMENT AND THE WATER

$$FSIP = KFIP \cdot \frac{SIP - IP}{KDOX} \qquad (g\ P/m^2/d)$$

DIFFERENTIAL EQUATIONS

The change in the state variable with time is calculated by adding all the processes together in a differential equation set up for each state variable.

Below the differential equations are defined:

$$\frac{dSON}{dt} = RSON - RSONNH - RESIM \qquad (g\ N/m^2/d)$$

$$\frac{dSNH}{dt} = \frac{RSONNH - RSNIT - FNH}{(1-DM)\cdot VF\cdot KDO2} \quad (g\ N/m^3/d)$$

$$\frac{dSNO3}{dt} = \frac{RSNIT - RDENIT - FNO3}{(1-DM)\cdot VF\cdot KDS} \quad (g\ N/m^3/d)$$

$$\frac{dSNIM}{dt} = RSNIN + RDENIT \quad (g\ N/m^2/d)$$

$$\frac{dSOP}{dt} = RSOP - ROPSIP - RSPIM \quad (g\ P/m^2/d)$$

$$\frac{dSIP}{dt} = \frac{-RFESIP + ROPSIP - FSIP}{(1-DM)\cdot VF\cdot KDS} \quad (g\ P/m^3/d)$$

$$\frac{dSPFE}{dt} = RFESIP \quad (g\ P/m^2/d)$$

$$\frac{dSPIM}{dt} = RSPIM \quad (g\ P/m^2/d)$$

APPENDIX F

PARAMETERS IN THE SEDIMENT SUBMODULE

The below tables include parameters for the N and P cycle, respectively.

Eutrophication Specifications, Sediment N	unit	Name	Suggested Value	References
Fraction of settled N mineralised on sediment		krsn0	0.2	0
Mineralisation of SON	1/h	krsn1	0.0001	BLACKBURN & HENRIKSEN (1983)
N:C ratio of immob. Org. N in sediment	g N/g C	knim	0.064	BLACKBURN & HENRIKSEN (1983)
Teta, mineralisation of SON in sediment		tetn	1.04	
Nitrification rate sediment	g N/m3/h	knit	0.1	LOMSTEIN (1995), RUADIJ & VAN RAAPHORST (1995), BLACKBURN & HENRIKSEN (1983)
Nitrificat. sediment, half satura. conc.	g N/m3	ksnh0	0.5	
Halfsaturation conc. for eelgrass uptake of SNH	g N/m3	ksen	0.9	BOCCI et al. (1997), COFFARO & BOCCI (1997), IZIUMI & HATTORI (1982)

Eutrophication Specifications, Sediment P	Unit	Name	Suggested Value	References
Teta for temperature, mineralisation of SOP		trsp	1.04	
Max. denit. sediment 20 C	g N/m3/h	demax	0.035	LOMSTEIN (1995)
Immobile P fraction of settled P		kpim	0.15	JENSEN et al. (1995)
Fraction of settled P mineralised at surface		krsp0	0.2	
Mineralisation of SOP	1/h	krsp1	0.0001	BLACKBURN & HENRIKSEN (1983)
Depth of active sediment layer	M	kds	0.1	User defined
Chemosorption of P to Fe+++	g P/g Fe	kfepo	0.066	MORTENSEN et al (1992), JENSEN et al. (1995), JACOBSEN (1977) & (1978)
Const. DO penetration in sediment	M	kka	0.00124	GUNDRESEN et al. (1995)
Const. DO penetration in sediment	m/DO	kkb	0.000403	GUNDRESEN et al. (1995)
Const. DO penetration in sediment	h*m3/DO	kkc	0.00132	GUNDRESEN et al. (1995)
Diffusion to from sed of SIP	m2/h	kfip	0.00001	LOMSTEIN (1995), SWEERTS et al. (1991)
Fe+++ conc. in surface sediment	g Fe/g DM	kfe		User defined
Dry weight sediment	g DM/g WW	dm		User defined
Mass/vol. of sediment	tonnes/m3	vf		User defined
Halfsaturation Fe+++ sorbtion of SIP	g P/m3	khfe	0.25	JACOBSEN (1977)
Rate for RFESIP	1/h	knap	0.001	RUADIJ & VAN RAAPHORST (1995),
Halfsat. conc. for EC uptake of SIP	g P/m3	ksep	0.05	
Diffusion of IN, SNH and SNO3 in sediment	m2/h	difn	0.0000096	LOMSTEIN (1995), SWEERTS et al. (1991)
Teta temp dependency of denitrification		tde	1.087	WINDOLF J et al. 1996

APPENDIX G

NOTATION OF PROCESSES IN THE SEDIMENT SUBMODULE

Notation	Sediment process	dimension
C	Concentration of NO3 in sediment	g NO3-N/m^3
DIFN	Diffusion of inorganic nitrogen in sediment	m^2/d
DM	Dry matter of sediment, specified by user	g DM/g
DNM3	Denitrification	g N/m^3/d
DO	O2 in water	g O2/m^3
Kd	Depth from KDO2 where NO3=0	M
KDO2	Layer with O2, se below	m
KDOX	Layer with NO3, see below	m
KDS	Depth of active sediment layer, specified by user	m
KKA	Min. O2 penetration	m
KKB	O2 dependent O2 penetration	m/g O2
KKC	Sed. respiration dependent O2 penetration	d*m^3/g O2
KNIM	N:C ratio below which no mineralization	g N/g C
KNIT	Potential nitrification at 20 C in sediment	g N/m^3/d
KRESN0	Fraction mineralised at 20 C	
KRESP0	Fraction mineralised at 20 C	
KRSN1	Mineralization rate SON	1/d
KRSP1	Mineralization rate SOP	1/d
KSNH0	Half saturation concentration for SNH	g N/m^3
MADE	Dept of water layer above sediment	m
MDO	Half saturation concentration for O2	g O2/m^3
ODSC	Total sediment O2 consumption	g O2/m^3/d
SEDC	Sedimentation of DC (detritus C)	g C/m^3/d
SEDN	Sedimentation of DN (detritus N),	g N/m^3/d
SEDP	Sedimentation of DP (detritus P)	g P/m^3/d
SEEC	Input to sediment of C in dead eelgrass, (option)	g C/m^3/d
SEEN	Input to sediment of N in dead eelgrass, (option)	g N/m^3/d
SEEP	Input to sediment of P in dead eelgrass, (option)	g P/m^3/d
SEPC	Sedimentation of PC (plankton C)	g C/m^3/d
SEPN	Sedimentation of PN (plankton N)	g N/m^3/d
SEPP	Sedimentation of PP (plankton P)	g P/m^3/d
$SPFE_{t-1}$	SPFE to time t-1	g P/m^2
TEMP	Water temperature	C
VF	Specific gravity, specified by user	g /cm^3
x	Sediment depth, x=0 at KDO2	m

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