Questions from the panel to the researchers

Introduction

The panel members have all read the report, and commented individually on it. In these first appraisals, all panel members have stressed the points that they thought were most important for the review. They have also raised a number of questions, that ranged from general discussion points to very specific questions asking for clarification, and details in need of closer examination.

Subsequently, the panel members have received the questions from the stakeholders. These questions also range from very general discussion points to detailed questions and comments. The general discussion points raised by the stakeholders corresponded well to the points already identified by the panel members. Some remarks are outside of the scope of the review (e.g. legal and economic issues) and will not be commented upon by the panel. Other issues are very local and also outside of the scope, as the panel members have insufficient knowledge to comment on them in detail. The final report of the panel will follow the structure of the scientific report and be formulated in general terms, but the panel intends to indicate in an appendix whether and how it responded to each of the stakeholder questions, and where this response is to be found in its report.

In this document the panel formulates a number of questions and discussion points to the researchers. A long and complicated report naturally raises questions and discussion points, as a large number of decisions have had to be made regarding the set-up of the study, choice of variables, indicators and processes, choice of policy measures etc. With the *general questions* formulated in this document we want to give the researchers the opportunity to better explain the reasoning behind these choices, where that was not clear to us in the report, or to justify the choices made. The panel wants to take into account these justifications wherever possible in its assessment. We consider these general questions to be the most important part of this document. In addition to these general questions, we also formulated a number of *detailed questions*. Sometimes these concern simple questions for clarification, sometimes they concern details that form part of the more general questions. We would appreciate a simple answer to these detailed questions, but expect that in many instances a reference to the answers to the general questions will suffice.

This document with questions, and the answers given to them, will not be published as part of the panel report. However, both documents will be archived as part of the underlying documentation of the panel report. The panel may cite (parts of) the answers in its final report, and will refer to these answers in an appropriate way.

General questions

Exclusive focus on reducing land-based N load to obtain good ecological status

Both the panel and the stakeholders miss a justification of the fundamental choice to focus exclusively on reduction of (diffuse) N sources as the main means to improve water quality. The situation is complex, as there is ample evidence that in many systems there is co-limitation of phytoplankton growth by N and P, with some seasonal pattern in most systems. In addition, N fixation in the Baltic may aggravate the problem and undo N reduction measures where ample P is available. But it is also true that the N:P ratio of winter loadings is biased towards N, and that historical reductions have affected P loadings much more than N loadings.

Questions:

We are in need of a thorough literature-based justification of the choices made, as this is a key aspect of the whole study and the policy.

In addition, we would like the researchers to answer the following questions:

- What data and evidence (published) exists that indicate which nutrient is limiting (N or P)?. This may vary with season and location (e.g. Baltic/North Sea). How does this address diverse water bodies?
- Nitrogen loading may be manageable, but is phosphorus in view of sediment exchange and large past efforts?
- In most systems, there is a gradual decrease in N loading that is not synchronous with the historical decrease in P loading. Which factors or policies have caused this decrease, and what is the expected autonomous trend in N loading under existing policies? Is there any quantitative information on this?
- How important is the *interaction* between N and P reductions and does the exclusive focus on N jeopardize the chances of reaching good status by the methods proposed here?
- Has N:P stoichiometry as a determining factor for phytoplankton composition been considered?
- Very important for the societal discussion: is the exclusive focus on (diffuse) N loading leading to the economically and societally optimal solution for the water quality problems? Is there evidence that it leads to the best results in comparison with the costs of the measures? Have any analyses been made of the cost aspects of the efforts required?
- apart from N-runoff from land (chosen as the primary concern) there are other factors that may affect Ecological Status. P loading has been mentioned. Also fisheries, habitat modification, change in the species composition of benthos have been mentioned in the literature, especially as influences on seagrass distribution. Have these factors been considered somehow, and is there evidence they are unimportant compared to land-based N runoff?
-

The adopted strategy to derive regionalized reduction targets for nutrient loading

In principle, nutrient reduction scenarios in a country can vary from a general, country-wide reduction target, over regionalized targets to water system specific targets. This document leads in the end to the definition of regional targets, but that comes as a surprise to the reader. The statistical modelling chapters suggested that water body specific targets would be defined, while the mechanistic model, based on country-wide reduction scenarios, suggested that one would arrive at a single national target. In the end, a regionalisation based on a set of aggregation rules were derived.

In general, there are arguments in favour of one national target (e.g. setting a level playing field for agriculture, simplicity of control, simplicity of communication, incorporating mutual influences between systems through coastal waters) but also in favour of specific targets (e.g. not overdoing efforts, optimal economic strategy). In the document, however, these arguments have not been made explicit and have not been the subject of extensive discussion.

Questions:

- procedural: when was it decided to adopt this regionalized strategy? Who decided this? Were the current scientific results used as a basis for this strategy? If so, how was this done precisely?
- How sure can we be that the regions are sufficiently homogeneous in their water bodies? In particular, when a regional target is low because most water bodies are open with short freshwater residence time, the region may also contain some sensitive, more isolated water bodies that would suffer from the low targets. Is this the case? How was it controlled?
- The scenarios used for the mechanistic modeling use boundary values that are (in part) determined by nation-wide reductions of nutrient loading with a certain percentage. If there are regions with mostly open water bodies and low reduction targets, the actual boundary conditions for all of these water bodies may differ from the modelled ones, since the reductions in the coastal area will be less. There is, thus, a discrepancy between the modeled policy and the actual policy. Will this affect the results of the study? Is it possible that the reduction strategy for these regions is too low, because it is the regional rather than the local reduction percentage that will influence the ecological status?

- The statistical modeling only focuses on within-system temporal trends and the causality in these trends. As far as we understand, no cross-system analysis, relating the hydrographical characteristics of the systems to their vulnerability to nutrient loading has been performed. Why hasn't this been done? It could have formed a scientific basis for the regionalisation, as well as a basis for investigating the sensitivity of the approach to within-region differences in water body characteristics?

Choice of indicators and their sensitivity to nutrient loading

Compared to the requirements of the WFD, only a limited set of indicators have been used. Only two of them (chlorophyll a and Kd) have been used across the two modelling approaches. This leaves a number of unstudied indicator variables with respect to the good ecological status:

- chl-a only gives an indication of phytoplankton biomass, not of composition. Thus it may miss occurrence of toxic blooms
- Kd is probably insufficient as an indicator of habitat quality for eelgrass. In particular, herbicide concentrations may be missed as an alternative explanatory variable. The literature on eelgrass in Denmark frequently mentions hysteresis and the occurrence of alternative stable states. It may be the case that low nutrient loading and high water transparency are necessary but insufficient conditions for eelgrass restoration - it would be very useful to bring forward quantitative arguments proving this point. However, it would still be needed to know what other factors contribute and how.
- The benthic index seems to be unresponsive and should be examined more closely or replaced
- nutrient stoichiometry (N:P in particular) is not considered
- toxic substances, in particular herbicides, might be needed as supporting physico-chemical variables

Questions:

- why are additional variables (e.g. days with nutrient limitation) used in the statistical modeling but not in the mechanistic modeling, especially as it appears that these variables correlate closely with chl-a and do not give much independent information?
- Could additional reference value targets be developed for TN and TP, using the same methodology as for chl-a? Presumably, these would be more directly related to loads and simpler to understand than the supplementary indicators used at present.
- None of the models has been able to show a strong influence of nutrient loading on Kd, except when going from hypertrophic to eutrophic conditions. Why is Kd nevertheless given more weight (at least with the statistical modeling) than other variables?
- what justifies the apparently arbitrary translation of calculated needed reductions (of N load in order to obtain target Kd) in the order of 200% to 25 %? Why 25 and not any other arbitrary number? Is the fact that unrealistic needed reductions are obtained, not a reason to decrease confidence in the models and downweight the importance of the variable in the final conclusions?
- What is the impact of the (doubtful) Kd calculations on the final results? Would the results have been essentially similar without these calculations or is the dependency (and thus the uncertainty) on Kd results large? This is important to estimate the robustness of the results!
- Can you derive supporting evidence from the literature that shows that nutrient loadings affect eelgrass independent of Kd, or that nutrients and Kd are necessary but insufficient conditions for eelgrass restoration?
- Have you considered other measures than nutrient load reduction in order to restore eelgrass beds?

Basic strategy of the statistical modeling

The statistical modeling focuses on within-system short-term models, resolving both long-term trends, seasonal variation and year-to-year variation that correlates with freshwater discharge. This is a choice, but

alternatives could have been chosen. One could have concentrated on long-term trends only, e.g. by correcting yearly values for freshwater discharge as is often done in Danish literature. One could also have chosen to model the cross-system differences as a function of hydrographic conditions (e.g. fraction freshwater in some form, stratification,…), thus enabling an evidence-based typology of systems, rather than the current (and unclear) basis for the typology. It would also have given an evidence base underlying the meta-modeling. At first sight, a long-term and cross-system approach would have fitted the purposes of the study better.

A second basic choice has been to detrend all independent variables, except the nutrient loadings, and not to detrend the response variables. This necessarily inflates the correlation between nutrient loadings and response variable, in case the latter shows trend: the trend can only be attributed to the nutrient loadings, also when in fact it would have been caused by climate change, increased freshwater extraction or other causes.

A third basic choice has been to select independent variables on MLS, and then apply regression models using PLS. This combines the sensitivity of MLS to colinearity in independent variables, and the bias in slope estimators (when applied for prediction) of PLS. The most important consequence of this choice is that only one nutrient loading can be selected, and combined effects of N and P loading, or their interaction, cannot be resolved by the models. Another consequence is that in some systems neither nutrient is selected as affecting the response variable, thus leading to a logical problem in estimating needed levels of reduction. Given the large knowledge on aquatic ecological processes, one wonders why variable selection has been needed in the first place, and why the modeling was not based on more advanced models that could have taken into account colinearity.

A final basic choice has been not to perform an explicit sensitivity analysis, or to report on the uncertainty of the results. Several methods to do this properly exist, both for within-system studies (e.g. based on Bayesian approach) and especially for between-system studies in a metamodeling or typology-based grouping of systems. Lack of communication about uncertainty of the findings hampers communication with stakeholders and induces risks of economic or ecological damage (in cases of overdoing, resp. underdoing).

Questions:

- Why has the choice been made for short-term, within-system models? Why are these better than alternatives?
- What justifies the choice for models that exclude the probing of interaction between different nutrients, one of the major problems in the current study?
- What justifies the variable selection procedure, given that the emphasis was not on proving the effects of nutrients on water quality, but the estimation of the regression coefficients?
- How reliable are the estimates of influence of nutrient loadings, given the strategy of detrending applied?
- Why have no measures of uncertainty been formally derived and presented in a way that is easy to understand for stakeholders? This could make the recommendations clearer and more acceptable. (e.g.https://www.ipcc.ch/pdf/supporting-material/uncertainty-guidance-note.pdf)
- (most important): What are consequences of all these choices for the conclusions?

Basic set-up and validation of the mechanistic models

In general, the model set-up is clear, but details of the processes and parameters are not easy to find, especially as some of the referred documents in the model description are not publicly available. In the general set-up, it is not entirely clear why in the end four different models were set up, especially as the use of a flexible mesh would have allowed to use a single model with spatially differing resolution. You mention in the description that the IDW model differs from the estuarine models in some process formulations and variable settings, and you give arguments why that has been done. We assume that you split the estuarine models in different models for practical reasons, but would like to know why. More importantly, we do not know if these models were the same in variables and parameters, and thus only differ from one another in bathymetry and boundary conditions. If settings differed, we would need details on the how and why.

Model validation was presented based on average values per month and water type. However, in the present setting a crucial validation element for the models is whether the models have been able to capture the long-

term trends in water quality as related to reductions in nutrients. Evidence showing the model behaviour in this respect should be easily obtainable from model output.

Questions:

- can you provide us with a copy of the documents you refer to in the model description?
- can you give more details on the four models, and what are their differences and similarities?
- can you specify details on the atmospheric forcing: was only a single year used, whereas Denmark reports on atmospheric deposition to Helcom for longer periods? How was the atmospheric N deposition divided over different species? Was atmospheric P deposition considered?
- can you provide us with the validation data showing that the models have been able to capture the essential effects of nutrient reduction on target variables chl-a and Kd?
- no estimates of model uncertainty were given. Do you have any estimate, what is it based on and what is the order of magnitude of the estimated error on the variables of interest (in particular the derived nutrient reduction need)?

Consistency between target values in statistical and mechanistic modeling

Both the statistical model chapters and the mechanistic model chapters describe how reference conditions and target values were defined. In the 'ensemble modeling', as well as in the meta-modeling, the targets from both model approaches are considered sufficiently consistent to be used in averaging procedures.

Questions:

- are these target and reference values conceptually consistent across the two modelling approaches? As far as we understand, the statistical modelling extrapolates back from the present situation in a particular water body to the situation that would be present if the *local* nutrient loading would be reduced to 1900 levels. This does not take into account the reduction in background marine values, nor the effect of local Danish reductions in other waters that reach the system of interest through the sea. It also does not take into account regional (e.g. BSAP) efforts. This reference value, therefore, must be significantly higher than the reference value calculated with the mechanistic model (which assumes both N and P reduction to 1900 levels, in both the system of interest and the whole world around). The reference value of the statistical model would be much closer to the '*target obtainable through Danish land-based N reduction*' in the mechanistic model. In terms of fig. 8.14: the intersection of the orange slope line with the upper dotted horizontal orange line, and not the point with the red cross. Can this relation between the definitions of the reference and target values be clarified, and can arguments be given why the approaches from both model strategies are nevertheless conceptually similar enough to be averaged?

Meta-modeling

While in general the strategy for meta-modeling is clear, there is a question regarding the North Sea waters on the Jutland coast, and a request from the panel for more supporting data.

Questions:

- can you explain how 'meta-modeled' results for North Sea waters could be derived, when none of the underlying models has considered this type of waters, which differ from all other water bodies in tidal range, temperature regime, sediment loading, nutrient concentration, stoichiometry and possibly a suite of other characteristics? Have the same indicators and criteria been used for North Sea and Baltic estuaries, and is this justified?
- A serious weakness of the report is that the input data basis is not sufficiently presented. Tables are lacking that show spatially resolved values for present and past atmospheric deposition, spatially resolved emission data from land, concrete concentrations in all rivers and estuaries for both N and P, and hydrographic data (e.g. % freshwater, residence time, tide, depth) for all

systems. The lack of area specific data does not allow a critical evaluation of regional MAI nor a comparison with data and results from other countries. The panel would greatly appreciate if such a table could be produced, preferably electronically.

Specific questions

Page	Report	Question
16		It seems formally strange to attribute F as "index" when it is a dimensional quantity (dimension L^3/T^2) and it does not appear very logical to divide runoff with residence time, that is, wouldn't a longer residence time imply larger runoff influence? Why not use a more straightforward parameter around specific freshwater content: f=R/(Q+R) = (Sm – S)/Sm
17	*Fig. 3.2*	Type 1 subtypes represent different nitrogen and phosphorus regimes, ranging from the quite Baltic Sea influenced to quite North Sea influenced, should perhaps this be taken into account in the model validation? On the other hand, the number of Type 1 areas that are both critically dependent on Danish nutrient inputs and significantly deviating from GES are probably limited.
20 / 58	*"In addition to the Danish land-based loadings, the mechanistic models also include N and P loadings at a regional scale, i.e. loadings to the entire Baltic Sea, and atmospheric deposition, see chapter 7."* and P 58: *"An important input to the setup of the mechanistic models is the external supply of nutrients. Apart from Danish land-based nutrient loadings, the mechanistic models include nutrient input to the Baltic Sea from other countries and atmospheric deposition. In section 4.2, Danish land-based nutrient loadings and atmospheric deposition are described, both based on data from the Danish monitoring programme DNAMAP."*	In shallow waters assumptions with respect to atmospheric deposition input can be crucial and potentially allow a manipulation of the MAI. Was the deposition data spatially resolved? If not, how was it taken into account in the model? Were gradients between land and sea taken into account? Which atmospheric N fractions were considered as bio-available in the model and how were they calculated? Was the atmospheric input of P fractions considered, as well?
24	*Time series of observatio ns (including Kd)*	How was Kd measured?
31	*"only time series with a minimum of 15 years were used"*	What is the statistical justification? How much data are omitted?
32	*"… refrained from doing so" (Log transformation)*	Are data normally distributed?
32	*"daily values gained from interpolation were used to construct monthly average values"*	Do you have a statistical reference for this procedure?
33	*"… we defined the following rules for predictor variables"*	Do you have statistical criteria or a reference for this? There are robust & complete time series analysis theories and methodologies available
37	*"The half saturation coefficients (Ks) for phosphorus and nitrogen were chosen to be 0.2 uM and 2 uM"*	What was the final weight of this exercise in the selection of variables?
41		Why did you not estimate error variances and confidence limits which are preconditions for evidence based, adaptive management, policy and decision making?
42	*"… quantification of autocorrelation , this effect was not included in the models"*	Your justification conflicts with your observation of significant autocorrelation, doesn't it?
52		calculation of Chl-a and KD is critical in this study. Thus, more information on how Chl-

		a is calculated from phytoplankton carbon and on the optical model parameterization relating model state-variables to KD would be interesting.
59	*„However, an important difference between the national data and the data adopted by AU for the mechanistic modelling is the resolution in time. Whereas the national data are reported on an annual basis, the data used for the modelling were provided on a daily basis, both for water discharges and nutrient loadings."*	How was this done?
59	*„The loadings were estimated as discharges of total nitrogen (TN) and total phosphorus (TP). Since the mechanistic models differentiate between the different chemical forms (inorganic/organic, dissolved/particulate, nitrogen and phosphorous species), the data were subsequently transformed into nutrient forms required by the modelling. Through an assessment of available observations on nutrients in water discharged from Danish catchments, monthly relations between inorganic and organic nutrients were developed and applied to split TN and TP into an inorganic and an organic fraction. By combining TOC and COD/BOD observations, the organic part was further split to separate the organic nutrients into the three forms adopted in the modelling process."*	Since the assumptions with respect of the model input are crucial for the later results, I like some clarifications. Am I right that you used (with respect to N) DIN and a part of TON as bio-available fractions in the model? How did you calculate it from biological and chemical oxygen demands (COD/BOD)? Did you take into account DON, as well? Was this calculated for every river separately or as an average for all Danish rivers? Could you give numbers about the relative share of each fraction for N and P?
59	*„Hence, the data are those officially reported by the various countries. Differentiation of TN and TP loadings was done according to Stepanauskas et al. (2002)." Stepanauskas et al. (2002): „We estimate that the input of summer riverine N to the Baltic Sea consists of 48% dissolved inorganic N, 41% DON, and 11% particulate N. Corresponding values for phosphorus are 46%, 18%, and 36% of dissolved inorganic P, DOP, and particulate P, respectively."*	Is this the same approach that you used for Danish rivers? Stepanauskas et al. (2002) quantify DIN and DON and these are the fraction you used as input for all other Baltic areas, is this right? In some areas the model seems not to cover the entire coast and nutrient retention may take place between river input and onset of the model domain. How did you deal with it?
60	*"… data were lumped according to topology…" Fig. 7.6*	Did you calibrate models by water body? Evaluation by type does not reveal accuracy and precision of water body specific models, does it? Would it be possible to estimate error variances and confidence limits (e.g. 0,95) for water body specific models? What are the estimated mean, covariance and variance of model parameters and error variances of water body specific models?
62	*Skills of biogeochemical models*	Is it true that all data was used for model calibration and that a model validation using an independent data set (year) was not carried out? In addition to regression coefficients demonstrating similar trends in model and data, can you also indicate that the actual values corresponded? Could you provide non-aggregated time series showing the model performance and data for concrete monitoring stations in comparison?
62	*"seasonal anoxia in these areas, inducing release of phosphorus from the sediments"*	Have the sorption-desorption on suspended sediment particles been taken into consideration?

61		What is the point of validation based on water body Type? Type 1 waters seem to include as diverse areas as the ones inside the sills to rather marine areas in Kattegat, why not use the different sub-categories of Type 1, Figure 3.2 and Table 8.1? How is the aggregation done into Type averages in e.g. Figure 7.6? Just mean value water bodies (model/observed data)? The quantitative assessment (page 65-66) is done on monthly mean time-series. That implies a mixture of validation of seasonal cycle and inter-annual variability. At least for the non-open water Types, it would make sense to explicitly look at the interannual variability that probably gives more information on the model's capabilities of resolving the response to load reductions.
76		The sediment pools are reduced for the reference simulation in the Baltic Sea and IDW based on literature values. But it is not explicitly stated whether this adaption resulted in a new quasi-steady-state in the model when forced with reference loads, which could be influential on several of the Type 1 water bodies. Is this the case?
77	*You attribute the decrease due to UWWT in Copenhagen, population about 600 000*	What management measures in the same time period have been implemented to treat the manure of the approx. 25million pigs? Each pig represents 3 person equivalents, so approximately 75 million people.
84	*"In order to reduce the influence of model bias, we used … ensemble models …" & "… most robust chlorophyll-a estimates were achieved using ensemble model"*	How can you justify this without proper error variance/uncertainty estimates?
87	*" … status values are converted into water body averages by relating the observed status to the modelled status at the actual observation point and applying the ratio between the two (model and observation) to correct the modelled water body average"*	Could you clarify? Are you correcting model results?
89	*"The purpose of averaging … is to reduce uncertainty"*	Can you justify? Is average any more certain than either of the models?
91		What is the method to estimate the weights? Could it be possible to use error variances of models as weights?
92	*"This choice is based on our wish from a management perspective to emphasise intercalibrated indicators and has no scientific basis"*	Does this mean the WFD intercalibration? Why does intercalibration not provide a scientific basis for the chosen indicators?
97	*"we chose a half saturation coefficient (Ks) for nitrogen limitation of 2 µM"*	On what basis (published) was this concentration chosen? This is difficult for a mix of diatoms, cyanobacteria and dinoflagellates.
92 *93* *94* *95*	*"… Kd indicator … are assigned double weight"* *"… light attenuation indicator has beem giving double weight"* *"… we have transformed the estimated PLR values into categories when above 25 %"*	All of these choices sound arbitrary and cursory. Can you justify?

96 *99* *99*	*"…due to the time constraints … we chose not to develop models" & "… the demand was assigned as 25 %.."* *"… values above one trigger a demand 25%"* *"we used categorization … as demonstrated in Table 8.7"* *"… the target values are rounded …"*	
102		The scenarios have the basis that BSAP nutrient load reductions are implemented. These comprise of massive P-load reductions (e.g., 60% for Baltic Proper that eventually should lead to halving winter DIP concentrations there), but all published scenarios show that the response time is quite slow with typical e-folding time of say 20 years. How is this time-delay handled in the model?
111		It is surprising that massive load reductions to Baltic Sea do not give more response to basin 217. The export of phosphorus from the Baltic proper should decrease substantially given that DIP concentrations should be reduced to 50% of present day concentrations in BSAP. Could you explain?
124	*"With respect to the North Sea water bodies, the data basis does not support the methodology described for mechanistic model-based meta model since biogeochemical modelling was not included in the study. However, GES has not been reached in any of the Danish water bodies in the North Sea and Skagerrak, and an approach taking limitation and differences into account has therefore been developed*	What is meant by this statement? It is unclear
125	*The described approach is subject to uncertainty.*	Can the uncertainty be expressed in a way that it is easily understoon by decision makers and stakeholders?
129	*"…95% confidence interval at +/- 13.5 % reduction"*	What can you say about model error variances and confidence limits based on the comparison of mechanistic and statistical models? Is this 13.5% the overall confidence interval of loading reduction?
130		Does the observation that for area 44 the statistical model fails because it does not take regional reductions into account imply that the statistical approach would fail for all Type 1 water bodies?
141	*"the methods presented here basically violate the one-out-all-out principle, which is defined when evaluating the ecological status and not when estimating measures to ensure GES"; "When reductions based on chlorophyll-a or Kd are averaged instead of choosing the maximum reductions,we do, in theory, not obtain GES for both indicators"*	Is the method therefore WFD compliant? If not, what is necessary to make it WFD compliant? What management measures are necessary to obtain GES for BOTH indicators?
141		It is stated that the basis is to obtain GES in 2027. This is fine, but it also has consequences on how to handle effects from regional reductions (BSAP), see the comment above on scenarios (page 102). It would be relevant to discuss the time aspect already in the beginning of the report as well, because we know the ecosystem responds slowly, and differently across the water bodies.

142	*"… focused on reducing uncertainties, for instance by averaging … and applying a type-specific approach*	You lose information at the same time. Can you guarantee reduction of uncertainties without proper statistical error analysis, that is, comparison on error variances of models based on actual and averaged data?
142	*"The ensemble model results reveal good agreement between the two very different model approaches …, thus indicating that the estimated MAIs are reliable"*	How can you say so without proper statistical error analysis?

MIKE
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DHI 3 Algae and Sediment Model

ECO Lab Template

Scientific Description

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CONTENTS

DHI 3 Algae and Sediment Model
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1 Introduction

ECO Lab is a numerical lab for Ecological Modelling. It is a generic and open tool for customising aquatic ecosystem models to describe for instance water quality and eutrophication. DHI's expertise and know how concerning ecological modelling has been collected in predefined ecosystem descriptions (ECO Lab templates) to be loaded and used in ECO Lab. So the ECO Lab templates describe physical, chemical and biological processes related to environmental problems and water pollution. The following is a description of the DHI 3 algae and sediment model.

The DHI 3 algae and sediment template is used in investigations of eutrophication effects where different algae species and sediment pools of nutrients are essential and as an instrument in environmental impact assessments for such ecosystems. The 3 algae and sediment modelling can be applied in environmental impact assessments considering:

- Pollution sources such as domestic and industrial sewage and agricultural run-off
- Cooling water outlets from power plants resulting in excess temperatures
- Physical conditions such as sediment loads and change in bed topography affecting especially the benthic vegetation
- Evaluation of action plans related to nutrient reductions
- Risk evaluation in connection to potential harmful algae blooms

The aim of using 3 algae and sediment modelling as an instrument in environmental impact assessment studies is to obtain, most efficiently in relation to economy and technology, the optimal solution with regards to ecology and the human environment.

The 3 algae and sediment model describes nutrient cycling including internal loadings from sediment pools of nutrient, phytoplankton and zooplankton growth, in addition to simulating oxygen conditions.

The model results describe the concentrations of phytoplankton, chlorophyll-a, zooplankton, organic matter (detritus), organic and inorganic nutrients, oxygen and the area-based sediment pools of nitrogen and phosphorous over time. In addition to this, a number of derived variables are stored: primary production, total nitrogen and phosphorus concentrations, sediment oxygen demand and Secchi disc depth.

The 3 algae and sediment template is integrated with the advection-dispersion module, which describes the physical transport processes at each grid-point covering the area of interest. Other data required are concentrations at model boundaries, flow and concentrations from pollution sources, water temperature and influx of light, etc.

2 Applications

The eutrophication template can be applied in a range of environmental investigations:

- Studies where the effects of alternative nutrient loading situations are compared and/or different waste water treatment strategies are evaluated.
- Studies of oxygen depletion.
- Studies of the effects of the discharge of cooling water.
- Comparisons of the environmental consequences of different construction concepts for harbours, bridges, etc.
- Evaluation of the environmental consequences of developing new urban and industrial areas.
- Evaluation of action plans related to nutrient reductions and long term effects of reduction scenarios.
- Risk evaluation in connection to potential harmful algae blooms.

3 Mathematical Formulations

The MIKE 21/3 ECO Lab is coupled to the MIKE 21/3 AD module in order to simulate the simultaneous processes of transport, dispersion and biological/biochemical processes.

The 3 algae and sediment model includes state variables for 3 pelagic algae groups, nutrients, oxygen, hydrogen sulphide and sediment pools of C, N and P as well as a number of sediment state variables..

Table 3.1 Pelagic state variables

Name	Comment	Unit
PC1	Flagellate C	g C m^{-3}
PC2	Diatom C	g C m^{-3}
PC3	Cyanobacteria C	g C m^{-3}
PN1	Flagellate N	g N m^{-3}
PN2	Diatom N	g N m^{-3}
PN3	Cyanobacteria N	g N m^{-3}
PP1	Flagellate P	g P m^{-3}
PP2	Diatom P	g P m^{-3}
PP 3	Cyanobacteria P	g P m^{-3}
Psi	Diatom Si	g Si m^{-3}
CH	Chlorophyll-a	g Chl m^{-3}
ZC	Zooplankton C	g C m^{-3}
DC	Detritus C	g C m^{-3}
DN	Detritus N	g N m^{-3}
DP	Detritus P	g P m^{-3}
DSi	Detritus Si	g Si m^{-3}
NH4	Total ammonia (NH_4)	g N m^{-3}
NO3	Nitrate+ nitrite	g N m^{-3}
H2S	Hydrogen Sulphide (H_2S)	g S m^{-3}
IP	Inorganic Phosphorous (PO_4)	g P m^{-3}
Si	Silicate Si	g Si m^{-3}
DO	Dissolved Oxygen	g O_2 m^{-3}
CDOC	Coloured refractory DOC	g C m^{-3}
CDON	Coloured refractory DON	g N m^{-3}
CDOP	Coloured refractory DOP	g P m^{-3}
LDOC	Labile DOC	g C m^{-3}
LDON	Labile DON	g N m^{-3}
LDOP	Labile DOP	g P m^{-3}

Table 3.2 Sediment state variables

Name	Comment	Unit
SSi	Sediment biological available Silicate	g Si m-2
KDOX	Oxidised layer, depth of NO3 penetration in sediment	m
KDO2	DO penetration into sediment	m
SOC	Sediment organic C	g C m-2
SON	Sediment organic N	g N m-2
SOP	Sediment organic P	g P m-2
FESP	Sediment iron adsorbed PO4	g P m-2
SNH	Sediment pore water NH4	g N m-2
SNO3	NO3-N in Surface sediment pore water, layer (0 - kdo2)	g N m-2
SIP	Sediment pore water PO4	g P m-2
SH2S	Sediment reduced substances as (H2S)	g S m-2
SPIM	Immobilised P in sediment	g P m-2
SNIM	Sediment immobilised N by denitrification & burial	g N m-2
SCIM	Sediment immobilised C by mineralisation & burial of SOC	g C m-2

Table 3.3 Additional State variables for mass considerations

Name	Comment	Unit
sum_PRPC	Sum of PC production	g C m-2
sum_CminW	Sum of pelagic C mineralisation	g C m-2
sum_minSOC	Sum of SOC mineralisation	g C m-2
sum_DEPON	Sum of atmospheric deposition of N	g N m-2
Sum_Nfix	Sum of cyanobaterial N fixation	g N m-2
sum_DENW	Sum of denitrification in water column	g N m-2
sum_Nflux	Sum of N flux sediment- water	g N m-2
sum_rdenit	Sum of sediment denitrification	g N m-2
sum_DEPOP	Sum of atmospheric deposition of P	g P m-2
sum_Pflux	Sum of P flux sediment-water	g P m-2
sum_rear	Sum of reaeration	g O2 m-2
sum_ODSC	Sum of sediment O2 respiration	g O2 m-2
sum_RSH2S	Sum of H2S production in sediment	g S m-2

The first 28 components or state variables (pelagic system) are moveable and treated in both the MIKE 21/3 AD and the MIKE 21/3 ECO Lab module. The additional components have a fixed nature belonging to the benthic system.

The processes and transfer of carbon, nitrogen and phosphorus in the Eutrophication model system is illustrated in Figure 3.1. Also included in the model is an oxygen balance.

The processes describing the variations of the components in time and space are dependent on external factors such as the salinity, water temperature, the light influx, and the discharges.

The salinity and water temperature can be results of MIKE 21/3 AD simulations or be user specified values. The first possibility is especially relevant for cooling water investigations whereas the latter possibility often is used in areas where only natural variations in temperature are seen.

The mathematical formulations of the biological and chemical processes and transformations for each state variable are described one by one below. The differential equations are 1st order, ordinary and coupled.

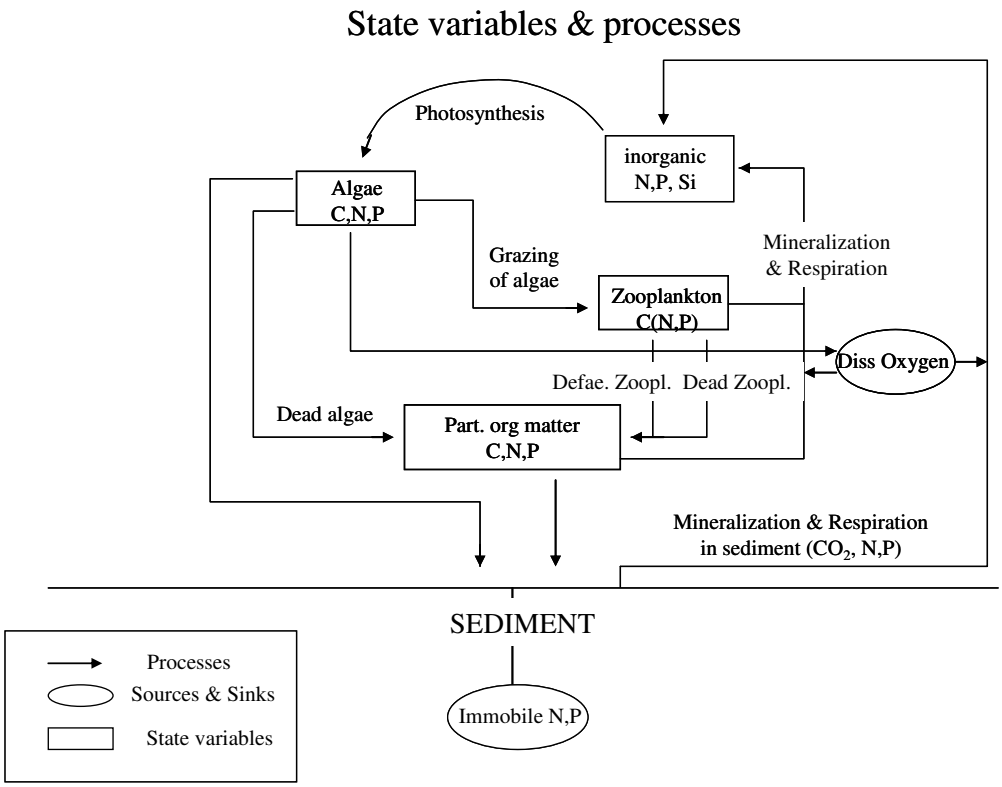

Figure 3.1 The simplified flow diagram of the fluxes of carbon, nitrogen and phosphorus in the eutrophication model.

3.1 Vertical light penetration

Light is essential for growth of all plants, including the pelagic. The vertical light penetration can be described by an exponential decay with depth which is dependent on a light extinction K_d, which either can be described as with light extinction constants (k_{dx}) multiplied by concentrations of light extinction concentration (Chlorophyll (CH, g m^{-3})), detritus (DC, g C m^{-3}), dissolved organic matter (CDOC, g C m^{-3}), inorganic matter (SS, g m^{-3}) and water($k_{bla,}$ m^{-1}) or it can be described as a function of scattering (b, m^{-1}) and absorption (a, m^{-1}) of light.

Vertical light penetration with depth (z, m) in the water column:

$$I_z = I_0 * e^{-K_{dx}*z} \text{ mol photons } m^2\ d^{-1} \quad (3.1)$$

Where K_{dx} can be either K_{d1} or K_{d2}:

$$K_{d1} = K_{chl} * CH + K_{dc} * DC + k_{cdoc} * CDOC + k_{ss} * SS + k_{bla}\ , m^{-1} \quad (3.2)$$

Or:

$$K_{d2} = \sqrt{a^2 + 0.256 * a * b}\ , m^{-1} \quad (3.3)$$

The absorption of light is mainly associated to particulate and dissolved organic matter whereas the scattering is mainly associated to particulate inorganic matter.

Light absorption, where the notation Kx_a stand for light absorption constant of component x:

$$a = K_{chl_a} * CH + K_{dc_a} * DC + K_{cdoc_a} * CDOC + K_{ss_a} * SS + k_{bla}\ , m^{-1} \quad (3.4)$$

Light scattering form phytoplankton and fine suspended inorganic matter can be describes as power functions of CH and SS:

$$b = bkch * CH^{ekch} + bkss * SS^{ekss}\ , m^{-1} \quad (3.5)$$

Where the light scattering constants (bkch, bkss in $m^2 g^{-1}$) and exponents (ekch, ekss) are for chlorophyll and inorganic suspended matter, respectively.

The present ecological model do not simulate resuspension of (fine) sediment, therefore SS is not dynamically simulated. Resuspension is most pronounced on shallow waters below 5-10 m. The user should therefore consider the need for either including measured SS concentrations or modelled concentrations of SS by a sediment transport model (MIKE by DHI 2011a). On shallow waters (like lagoons) the EU-MT ECO Lab template can be used. This template includes resuspension of and transport of fine sediment and combine it with a description of nutrients (N, P) one phytoplankton group, one macroalgae, one rooted macrophyte (eelgrass) and microbenthic algae (Rasmussen E. K. et al. 2009).

The present model however calculates dynamically the concentration of chlorophyll (CH), detritus carbon (DC) and refractory or coloured dissolved organic C (CDOC). The missing resuspension of SS is minimal if used on set up with waters above 10 m depth, like the Baltic Sea.

3.2 Production of autotrophs

The template includes 3 pelagic autotrophs (flagellates, diatoms and cyanobacteria). The production is based on daily dose of photosynthetic active light (PAR, mol photons m^2d^{-1}) light resulting in a net production.

The differential equation includes a net production, sedimentation, buoyancy (flagellate & cyanobacteria) and mortality by grazing and nutrient limitation (nutrient stress).

$$\frac{dX}{dt} = gross\ production - mortality - sedimentation + \ boyancy \tag{3.6}$$

The net production is determined by light (*flight(i)*), temperature (*ftemp(T)*) and nutrient availability (*fnut(N,P, (Si diatoms))*). μ_T is the temperature corrected max specific growth (d^{-1}) and X is the biomass (g C m^{-3} or g C m^{-2})

$$net\ production = \mu_T * flight(i) * ftemp(T) * fnut\big(N, P, (Si)\big) * FAC * RD * X \tag{3.7}$$

Where:

Name	Comment	Unit
μ	Max specific net growth rate (12 h light/12 h dark) at 20 °C	d^{-1}
i	Light (PAR) dose	mol photon m^{-2} d^{-1}
T	Temperature	°C
N,P, Si	Internal concentrations of N, P and SI in algae	g nutrient g C^{-1}
FAC	Correction of dark reaction (growth)	n.u.
RD	Relative day length, function of latitude, 1 at 12 h light	n.u

Temperature is an important direct or indirect regulator of many processes. Two types of temperature functions are used, Arrhenius or Lassiter functions.

The Arrhenius function increases the process exponentially with temperature; whereas the Lassiter function have an optimum temperature from which the process decline towards zero.

In the present template Arrhenius relations are used to describe the max specific growth rates, as the template is used in waters where the temperature rarely exceeds 20 °C. Further at increasing temperatures the plankton community will have a tendency to adapt to the higher temperature by change of species composition.

The user is encouraged to consider the feasibility to change from Arrhenius to a Lassiter temperature regulation of the max specific growth rates if needed. Both Arrhenius and Lassiter expressions are bullied in function in ECO Lab see (MIKE by DHI 2011b).

Lassiter functions are used to temperature regulate the max specific growth rates. In contrast to the Arrhenius function The Lassiter function include an optimum temperature above which the function will decline. Arrhenius functions are used to regulate the specific growth of phytoplankton or macrophytes in areas normally having summer temperatures well above 20 °C.

It is still recommended to use Arrhenius functions for temperature regulation of respiration processes; however the user might consider to increase the reference temperature for 20 °C, if data or references justify this.

Lassiter:

$$L(T) = p_{opt} * e^{K2*(T-T_{opt})} * \left(\frac{(T_{max}-T)}{(T_{max}-T_{opt})}\right)^{K2*(T_{max}-T_{opt})}, d^{-1} \quad (3.8)$$

Arrhenius 20 °C:

$$A(T) = \theta^{(T-20)}, d^{-1} \quad (3.9)$$

Where:

T:	Temperature °C
popt:	max growth at Topt, d-1
Topt:	Optimum temperature °C
Tmaxt:	Maximum temperature° C
Θ:	Teta constant Arrhenius function
K2:	constant

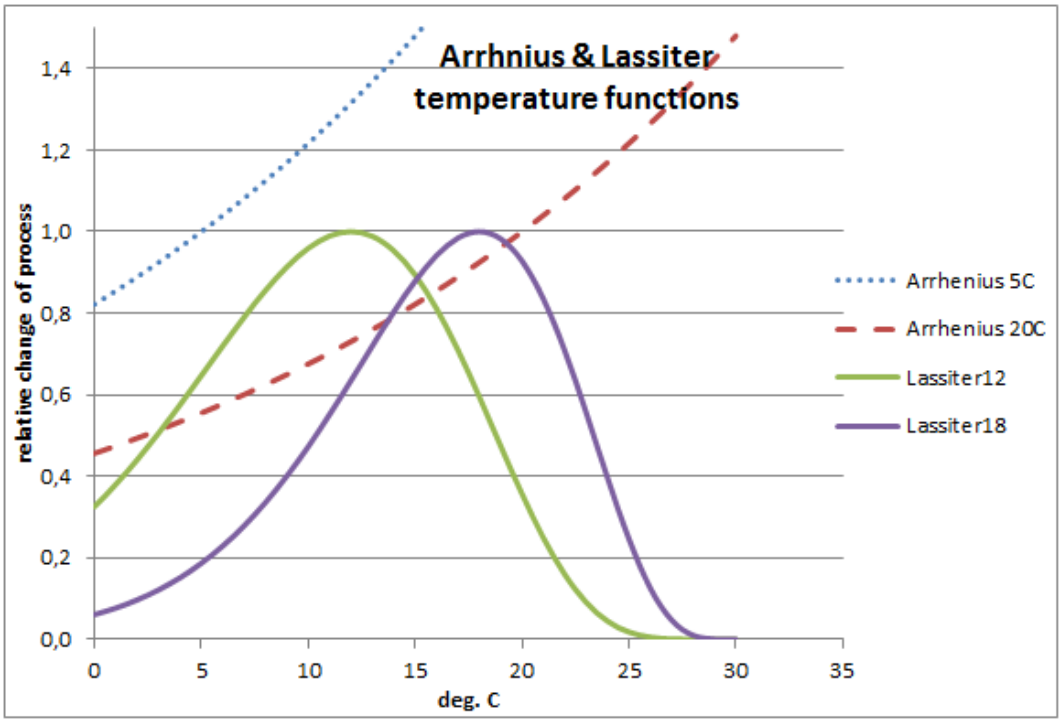

Figure 3.2 Arrhenius at 5 and 20 °C (Θ 1.04) and Lassiter function at T_{opt} at 12 and 18 °C (T_{max} 30 °C, K2 0.4)

The nutrient regulates the growth of all autotrophs. Two different nutrient regulators of the growth are used. A Droop kinetic (Droop 1973, Droop 1975) is used for autotrophs having internal nutrient pools (flagellates, diatoms, cyanobacteria). A Monod kinetics (Monod J. 1949) is used to describe the uptake of inorganic N, P and Si from the water into plankton.

Further cyanobacteria has the ability to N fixation in situation where the internal N:C ratio is low and the internal P:C is above average.

Nutrient regulation of primary production of phytoplankton (flagellates and cyanobacteria):

$$fnut(N,P)_{pm} = \frac{2}{\frac{1}{f(N)_{pm}} + \frac{1}{f(P)_{pm}}} \tag{3.10}$$

In the expression for diatoms Si is included:

$$fnut(N,P,Si)_{pm} = \frac{3}{\frac{1}{f(N)_{pm}} + \frac{1}{f(P)_{pm}} + \frac{1}{f(Si)_{pm}}} \tag{3.11}$$

Droop kinetics used for N modified after (Nyholm1978, Nyholm 1979) is used to regulate growth of phytoplankton:

$$f(N)_{pm} = \frac{\frac{PN}{PC} - PNmin}{PNmax - PNmin} \tag{3.12}$$

The same formulation is used for diatoms.

Droop kinetics used for P modified after (Nyholm1978, Nyholm 1979) is used to regulate growth of phytoplankton:

$$f(P)_{pm} = \frac{\left(\frac{PP}{PC} - PPmin\right) * (Kc + PPmax - PPmin)}{(PPmax - PPmin) * (Kc + \frac{PP}{PC} - PPmin)} \tag{3.13}$$

Where:

Name	Comment	Unit
PC	Phytoplankton C	g C m-3
PN	Phytoplankton N	g N m-3
PP	Phytoplankton P	g P m-3
PNmin	Minimum N:C ratio for phytoplankton	g N g C-1
PNmax	Maximum N:C ratio for phytoplankton	g N g C-1
PPmin	Minimum P:C ratio for phytoplankton	g P g C-1
PPmax	Maximum P:C ratio for phytoplankton	g P g C-1

3.3 Differential equations pelagic state variables

3.3.1 PC1: Flagellate C, g C m^{-3}

$$dPC1/dt = PRPC1 - GRPC1 - DEPC1 - SEPC1 - BUOYC1 \quad (3.14)$$

Where:

Process	Comment	Unit
PRPC1	Net production flagellate carbon	g C m^{-3} d^{-1}
GRPC1	Grazing of flagellate carbon	g C m^{-3} d^{-1}
DEPC1	Death of flagellate carbon	g C m^{-3} d^{-1}
SEPC1	Settling of flagellate carbon	g C m^{-3} d^{-1}
BUOYC	Flagellate upward movement	g C m^{-3} d^{-1}

PRPC1: Net Production flagellate carbon, g C m^{-3} d^{-1}

$$PRPC1 = mntp1 * myfi1 * fac * rd * PC1 \quad (3.15)$$

Where:

Name	Comment	Unit	Type*)
mntp1	N, P & temperature corrected max. net growth rate	d^{-1}	A
myfi1	Light function Flagellate,	n.u.	A
fac	Phytoplankton, Correction for dark reaction	n.u.	C
rd	Relative daylength, f(latitude, day,month,year)	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

GRPC1: Grazing of phytoplankton (Flagellate) carbon, g C $m^{-3}d^{-1}$

$$GRPC1 = \frac{kedib1 * MAX(PC1 - 0.001)}{MAX(0.001, kedib1 * PC1 + kedib2 * PC2 + kedib3 * PC3)} * mgpc * zc \quad (3.16)$$

Where:

Name	Comment	Unit	Type*)
Kedib1	Edible fraction of Flagellate	n.u.	C
Kedib2	Edible fraction of Diatoms	n.u.	C
Kedib3	Edible fraction of Cyanobacteria	n.u.	C
PC1	Flagellate C	g C m^{-3}	S
PC2	Diatom C	g C m^{-3}	S
PC3	Cyanobacterie C	g C m^{-3}	S
mgpc	Temperature & food corrected grazing rate	d^{-1}	A
ZC	Zooplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

DEPC1: Death of phytoplankton (flagellate) carbon, g C $m^{-3}d^{-1}$

$$DEPC1 = kdma * mnl1 * PC1 \quad (3.17)$$

Where:

Name	Comment	Unit	Type*)
kdma	Specific death rate phytoplankton	d^{-1}	C
mnl1	Nutrient dependent death factor, flagellate	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

SEPC1: Settling of phytoplankton (flagellate) carbon, g C $m^{-3}d^{-1}$
Phytoflagellates has the ability of vertical movement in the water column optimising their ability to pick up nutrient and gain light. During nutrient limitation the flagellates is assumed to seek down to the pycnocline to pick up nutrient, and in case they are not nutrient limited they are assumed to stay in the photic zone.

In the present model nutrient limitation, in term of a low PN/PC and or PP/PC ratio, enhance the sedimentation rate. PN/PC and PP/PC ratios close to maximum N and P content in the algae result in a reduction of the sedimentation rate. The nutrient regulation of the sedimentation rate is expressed in the auxiliary ***sed1***.

Light is also regulating the sedimentation rate. At high light dozes the sedimentation is accelerated at medium light dozes sedimentation is ***mspc1*** and at low light dozes the sedimentation decreases. This light regulation is expressed in the auxiliary ***fiz***.

$$SEPC1 = \frac{mspc1}{dz} * sed1 * fiz * PC1 \quad (3.18)$$

Where:

Name	Comment	Unit	Type*)
mspc1	Sedimentation rate flagellate phytoplankton	m d^{-1}	A
Dz	Height of actual water layer	m	F
sed1	N & P regulation of sedimentation. flagellate	n.u.	A
Fiz	Light factor for PC1 & PC3 sedimentation	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

BUOYC1: Flagellate upward movement, g C $m^{-3}d^{-1}$
The vertical upward movement by the phytoflagellates is described as a function of light doze and the algae's nutrient condition expressed in the auxiliary *buoy1*. An upward vertical movement is enhanced by a good nutrient condition and a low light doze.

$$BUOYC1 = \frac{mspc1 * buoy1 * PC1}{dz} \quad (3.19)$$

Where:

Name	Comment	Unit	Type*)
mspc1	Sedimentation rate flagellate phytoplankton	m d^{-1}	A
buoy1	N & P & light upward movement function, flagellate	n.u.	A
Dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.2 PC2: Diatom C, g C m^{-3}

$$\frac{dPC2}{dt} = PRPC2 + GRPC2 - DEPC2 - SEPC2 \quad (3.20)$$

Where:

Process	Comment	Unit
PRPC2	Net production diatom carbon	g C m^{-3} d^{-1}
GRPC2	Grazing of diatom carbon	g C m^{-3} d^{-1}
DEPC2	Death of diatom carbon	g C m^{-3} d^{-1}
SEPC2	Settling of diatom carbon	g C m^{-3} d^{-1}

PRPC2: Net Production phytoplankton carbon, g C $m^{-3}d^{-1}$

$$PRPC2 = mntp2 * myfi * fac * rd * PC2 \quad (3.21)$$

Where:

Name	Comment	Unit	Type*)
mntp2	N, P, Si & temperature corrected max. net growth rate	d^{-1}	A
myfi2	Light function Diatom	n.u.	A
fac	Phytoplankton, correction for dark reaction	n.u.	C
rd	Relative daylength, f(latitude, day,month,year)	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

GRPC2: Grazing of phytoplankton (Diatom) carbon, g C $m^{-3}d^{-1}$

$$GRPC2 = \frac{kedib2 * MAX(PC2 - 0.001)}{MAX(0.001, kedib1 * PC1 + kedib2 * PC2 + kedib3 * PC3)} * mgpc * zc \quad (3.22)$$

Where:

Name	Comment	Unit	Type*)
Kedib1	Edible fraction of Flagellate	n.u.	C
Kedib2	Edible fraction of Diatoms	n.u.	C
Kedib3	Edible fraction of Cyanobacteria	n.u.	C
PC1	Flagellate C	g C m^{-3}	S
PC2	Diatom C	g C m^{-3}	S
PC3	Cyanobacterie C	g C m^{-3}	S
mgpc	Temperature & food corrected grazing rate	d^{-1}	A
ZC	Zooplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

DEPC2: Death of diatom carbon, g C $m^{-3}d^{-1}$

$$DEPC2 = kdma * mnl2 * PC2 \quad (3.23)$$

Where:

Name	Comment	Unit	Type*)
kdma	Specific death rate phytoplankton	d^{-1}	C
mnl2	Nutrient dependent death factor, diatom	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

SEPC2: Settling ofdiatom carbon, g C $m^{-3}d^{-1}$

$$SEPC2 = mspc2 * \frac{mnl2}{dz} * PC2 \quad (3.24)$$

Where:

Name	Comment	Unit	Type*)
mspc2	Sedimentation rate diatom phytoplankton	m d^{-1}	A
mnl2	Nutrient function, sedimentation & death, diatom	n.u.	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.3 PC3: Cyanobacteria C, g C m^{-3}

$$dPC3/dt = PRPC3 - GRPC3 - DEPC3 - SEPC3 - BUOYC3 \quad (3.25)$$

Where:

Process	Comment	Unit
PRPC3	Net production cyanobacteria carbon	g C m-3 d-1
GRPC3	Grazing of cyanobacteria carbon	g C m-3 d-1
DEPC3	Death of cyanobacteria carbon	g C m-3 d-1
SEPC3	Settling of cyanobacteria carbon	g C m-3 d-1
BUOYC3	Cyanobacteria upward movement	g C m-3 d-1

PRPC3: Net Production cyanobacteria carbon, g C $m^{-3}d^{-1}$

$$PRPC3 = mntp3 * myfi3 * fp3sal * fac * rd * PC3 \quad (3.26)$$

Where:

Name	Comment	Unit	Type*)
mntp3	N, P & temperature corrected max. net growth rate	d^{-1}	A
myfi3	Light function Cyanobacteria,	n.u.	A
fp3sal	Function for cyanobacteria dependency of salinity	n.u.	A
fac	Cyanobacteria, Correction for dark reaction	n.u.	C
rd	Relative daylength, f(latitude, day,month,year)	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

GRPC3: Grazing of cyanobacteria (Flagellate) carbon, g C $m^{-3}d^{-1}$

$$GRPC3 = \frac{kedib3 * MAX(PC3 - 0.001)}{MAX(0.001, kedib1 * PC1 + kedib2 * PC2 + kedib3 * PC3)} * mgpc * zc \quad (3.27)$$

Where:

Name	Comment	Unit	Type*)
Kedib1	Edible fraction of Cyanobacteria	n.u.	C
Kedib2	Edible fraction of Diatoms	n.u.	C
Kedib3	Edible fraction of Cyanobacteria	n.u.	C
PC1	Flagellate C	g C m^{-3}	S
PC2	Diatom C	g C m^{-3}	S
PC3	Cyanobacteria C	g C m^{-3}	S
mgpc	Temperature & food corrected grazing rate	d^{-1}	A
ZC	Zooplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

DEPC3: Death of cyanobacteria carbon, g C $m^{-3}d^{-1}$

$$DEPC3 = kdma * \frac{mnl3}{fp3sal} * PC3 \quad (3.28)$$

Where:

Name	Comment	Unit	Type*)
kdma	Specific death rate cyanobacteria	d^{-1}	C
mnl3	Nutrient dependent death factor, cyanobacteria	n.u.	A
fp3sal	Function for cyanobacteria dependency of salinity	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

SEPC3: Settling of cyanobacteria carbon, g C $m^{-3}d^{-1}$

Cyanobacteria has the ability of vertical movement in the water column optimising their ability to pick up nutrient and gain light. During nutrient limitation the cyanobacteria seek down to the pycnocline to pick up P nutrients, and in case they are not nutrient limited (P) they are assumed to stay in the photic zone.

In the present model nutrient limitation, in term of a low PN/PC and or PP/PC ratio, enhance the sedimentation rate. PN/PC and PP/PC ratios close to maximum N and P content in the algae result in a reduction of the sedimentation rate. The nutrient regulation of the sedimentation rate is expressed in the auxiliary ***sed3.***

Light is also regulating the sedimentation rate. At high light dozes the sedimentation is accelerated at medium light dozes sedimentation is ***mspc3*** and at low light dozes the sedimentation decreases. This light regulation is expressed in the auxiliary ***fiz***.

$$SEPC3 = \frac{mspc3}{dz} * sed3 * fiz * PC3 \quad (3.29)$$

Where:

Name	Comment	Unit	Type*)
mspc3	Sedimentation rate cyanobacteria	m d^{-1}	A
Dz	Height of actual water layer	m	F
sed3	N & P regulation of sedimentation. cyanobacteria	n.u.	A
Fiz	Light factor for PC1 & PC3 sedimentation	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

BUOYC3: Cyanobacteria upward movement, g C $m^{-3}d^{-1}$
The vertical upward movement by the cyanobacteria is described as a function of light doze and the algae's nutrient condition expressed in the auxiliary ***buoy3***. An upward vertical movement is enhanced by a good nutrient condition and a low light doze.

$$BUOYC3 = \frac{mspc3 * buoy3 * PC3}{dz} \quad (3.30)$$

Where:

Name	Comment	Unit	Type*)
mspc3	Sedimentation rate cyanobacteria	d^{-1}	A
Buoy3	N & P & light upward movement function, cyanobacteria	n.u.	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.4 PN1: Flagellate N, g N m^{-3}

$$\frac{dPN1}{dt} = UPNH1 + UPN31 - GRPN1 - DEPN1 - SEPN1 - BUOYN1 \quad (3.31)$$

Where:

Process	Comment	Unit
UPNH1	Uptake of NH_4 into flagellates N	g N m^{-3} d^{-1}
UPN31	Uptake of NO_3 into flagellates N	g N m^{-3} d^{-1}
GRPN1	Grazing of flagellates N	g N m^{-3} d^{-1}
DEPN1	Death of flagellates N	g N m^{-3} d^{-1}
SEPN1	Settling of flagellates N	g N m^{-3} d^{-1}
BUOYN1	Upward movement flagellate N	g N m^{-3} d^{-1}

UPNH1: Uptake of NH_4 into flagellate N, g N m^{-3} d^{-1}

$$UPNH1 = MIN(unh1, pnma * PRPC1) \quad (3.32)$$

UPN31: Uptake of NO_3 into flagellate N, g N m^{-3} d^{-1}

$$UPN31 = MAX(0, MIN(un31, pnma * PRPC1 - UPNH1)) \quad (3.33)$$

GRPN1: Grazing of flagellate N, g N m^{-3} d^{-1}

$$GRPN1 = pn1pc1 * GRPC1 \quad (3.34)$$

DEPN1: Death of flagellate N, g N m^{-3} d^{-1}

$$DEPN1 = pn1pc1 * DEPC1 \quad (3.35)$$

SEPN1: Settling of flagellate N, g N m^{-3} d^{-1}

$$SEPN1 = pn1pc1 * SEPC1 \quad (3.36)$$

BUOYN1: Upward movement of PN1, g N m^{-3} d^{-1}

$$BUOYN1 = pn1pc1 * BUOYC1 \quad (3.37)$$

Where:

Name	Comment	Unit	Type*)
pnma	Max. intracellular algae N	g N g C^{-1}	C
unh1	potential NH_4 uptake by flagellate	g N m^{-3} d^{-1}	A
un31	potential NO_3 uptake by flagellate	g N m^{-3} d^{-1}	A
pn1pc1	Flagellate N:C ration	g N g C^{-1}	A
PC1	Flagellate C	g C m^{-3}	S
GRPC1	Grazing of flagellate C	g C m^{-3} d^{-1}	P
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
SEPC1	Settling of flagellate C	g C m^{-3} d^{-1}	P
BUOYC1	Upwared movement of flagellate C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.5 PN2, Diatom N, g N m^{-3}

$$\frac{dPN2}{dt} = UPNH2 + UPN32 - GRPN2 - DEPN2 - SEPN2 \quad (3.38)$$

Where:

Process	Comment	Unit
UPNH2	Uptake of NH_4 into diatoms N	g N m^{-3} d^{-1}
UPN32	Uptake of NO_3 into diatoms N	g N m^{-3} d^{-1}
GRPN2	Grazing of diatoms N	g N m^{-3} d^{-1}
DEPN2	Death of diatoms N	g N m^{-3} d^{-1}
SEPN2	Settling of diatoms N	g N m^{-3} d^{-1}

UPNH2: Uptake of NH_4 into diatom N, g N m^{-3} d^{-1}

$$UPNH2 = MIN(unh2, pnma * PRPC2) \quad (3.39)$$

UPN32: Uptake of NO_3 into diatom N, g N m^{-3} d^{-1}

$$UPN32 = MAX(0, MIN(un32, pnma * PRPC2 - UPNH2)) \quad (3.40)$$

GRPN2: Grazing of dioatom N, g N m^{-3} d^{-1}

$$GRPN2 = pn2pc2 * GRPC2 \quad (3.41)$$

DEPN2: Death of diatom N, g N m^{-3} d^{-1}

$$DEPN2 = pn2pc2 * DEPC2 \quad (3.42)$$

SEPN2: Settling ofdiatom N, g N m^{-3} d^{-1}

$$SEPN2 = pn2pc2 * SEPC2 \quad (3.43)$$

Where:

Name	Comment	Unit	Type*)
pnma	Max. intracellular algae N	g N g C $^{-1}$	C
unh2	potential NH_4 uptake by diatom	g N m^{-3} d^{-1}	A
un32	potential NO_3 uptake by diatom	g N m^{-3} d^{-1}	A
pn2pc2	Diatom N:C ration	g N g C^{-1}	A
PC2	Diatom C	g C m^{-3}	S
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
SEPC2	Settling of diatom C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.6 PN3, Cyanobacteria N, g N m^{-3}

$$\frac{dPN3}{dt} = UPNH3 + UPN33 + NFIX - GRPN3 - DEPN3 - SEPN3 - BUOYN3 \quad (3.44)$$

Where:

Process	Comment	Unit
UPNH3	Uptake of NH_4 into cyanobacteria N	g N m^{-3} d^{-1}
UPN33	Uptake of NO_3 into cyanobacteria N	g N m^{-3} d^{-1}
NFIX	N fixation cyanobacteria	g N m^{-3} d^{-1}
GRPN3	Grazing of cyanobacteria N	g N m^{-3} d^{-1}
DEPN3	Death of cyanobacterias N	g N m^{-3} d^{-1}
SEPN3	Settling of cyanobacterias N	g N m^{-3} d^{-1}
BUOYN3	Upward movement cyanobacteria N	g N m^{-3} d^{-1}

UPNH3: Uptake of NH4 into cyanobacteria N, g N m^{-3} d^{-1}

$$UPNH3 = MIN(unh3, pnma * PRPC3) \quad (3.45)$$

UPN33: Uptake of NO3 into cyanobacteria N, g N m^{-3} d^{-1}

$$UPN33 = MAX(0, MIN(un33, pnma * PRPC3 - UPNH3)) \quad (3.46)$$

NFIX: N fixation by cyanobacteria N, g N m^{-3} d^{-1}

$$NFIX = IF\ (krednc - pn3pc3) < epsi\ THEN\ 0\ ELSE$$
$$knfix1 * tppc^{T-20} * \frac{MAX(0, krednp - pn3pc3)}{MAX(0, krednp - pn3pc3) + kqppn} * nfix1 * nfix2 \quad (3.47)$$

GRPN3: Grazing of cyanobacteria N, g N m^{-3} d^{-1}

$$GRPN3 = pn3pc3 * GRPC3 \quad (3.48)$$

DEPN3: Death of cyanobacteria N, g N m^{-3} d^{-1}

$$DEPN3 = pn3pc3 * DEPC3 \quad (3.49)$$

SEPN3: Settling of cyanobacteria N, g N m^{-3} d^{-1}

$$SEPN3 = pn3pc3 * SEPC3 \quad (3.50)$$

BUOYN3: Upward movement of PN3, g N m^{-3} d^{-1}

$$BUOYN3 = pn3pc3 * BUOYC3 \quad (3.51)$$

Where:

Name	Comment	Unit	Type*)
Pnma	Max. intracellular algae N	g N g C $^{-1}$	C
unh3	potential NH_4 uptake by cyanobacteria	g N m^{-3} d^{-1}	A
un33	potential NO_3 uptake by cyanobacteria	g N m^{-3} d^{-1}	A
pn3pc3	Cyanobacteria N:C ration	g N g C^{-1}	A
krednc	Redfield ratio N:C	g N g C^{-1}	C
knfix1	Max. N fixation, 20 °C, cyanobacteria	g N g C^{-1}d^{-1}	C
Tppc	Θ in Arrhenius temperature function	n.u.	C
T	Temperature	°C	F
Kqppn	Half saturation constant, N fixation	g N g C^{-1}	C
nfix1	Function for N fixation (1 if PSU≤12 else 0)	n.u.	A

Name	Comment	Unit	Type*)
nfix2	Function for N fixation (1 if 0≤PSU≤10 else 0-1)	n.u.	A
PC3	Cyanobacteria C	g C m^{-3}	S
GRPC3	Grazing of cyanobacteria C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
SEPC3	Settling of cyanobacteria C	g C m^{-3} d^{-1}	P
BUOYC3	Upwared movement of cyanobacteria C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.7 PP1, Flagellate P, g P m^{-3}

$$\frac{dPP1}{dt} = UPPP1 - GRPP1 - DEPP1 - SEPP1 - BUOYP1 \quad (3.52)$$

Where:

Process	Comment	Unit
UPPP1	Uptake of PO_4 into flagellates P	g P m^{-3} d^{-1}
GRPP1	Grazing of flagellates P	g P m^{-3} d^{-1}
DEPP1	Death of flagellates P	g P m^{-3} d^{-1}
SEPP1	Settling of flagellates P	g P m^{-3} d^{-1}
BUOYP1	Upward movement flagellate	g P m^{-3} d^{-1}

UPPP1: Uptake of PO4 into flagellate P, g P m^{-3} d^{-1}

$$UPPP1 = MIN(upo1, ppma * PRPC1) \quad (3.53)$$

GRPP1: Grazing of flagellate P, g P m^{-3} d^{-1}

$$GRPP1 = pp1pc1 * GRPC1 \quad (3.54)$$

DEPP1: Death of flagellate P, g P m^{-3} d^{-1}

$$DEPP1 = pp1pc1 * DEPC1 \quad (3.55)$$

SEPP1: Settling of flagellate P, g P m^{-3} d^{-1}

$$SEPP1 = pp1pc1 * SEPC1 \quad (3.56)$$

BUOYP1: Upward movement of PP1, g P m^{-3} d^{-1}

$$BUOYP1 = pp1pc1 * BUOYC1 \quad (3.57)$$

Where:

Name	Comment	Unit	Type*)
pnma	Max. intracellular algae P	g P g C^{-1}	C
upo1	Potential PO_4 uptake by flagellate	g P m^{-3} d^{-1}	A
pp1pc1	Flagellate P:C ration	g P g C^{-1}	A
PC1	Flagellate C	g C m^{-3}	S
GRPC1	Grazing of flagellate C	g C m^{-3} d^{-1}	P
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
SEPC1	Settling of flagellate C	g C m^{-3} d^{-1}	P
BUOYC1	Upward movement of flagellate C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.8 PP2, Diatom P, g P m^{-3}

$$\frac{dPP2}{dt} = UPPP2 - GRPP2 - DEPP2 - SEPP2 \quad (3.58)$$

Where:

Process	Comment	Unit
UPPP2	Uptake of PO_4 into diatoms P	g P m^{-3} d^{-1}
GRPP2	Grazing of diatoms P	g P m^{-3} d^{-1}
DEPP2	Death of diatoms P	g P m^{-3} d^{-1}
SEPP2	Settling of diatoms P	g P m^{-3} d^{-1}

UPPP2: Uptake of PO4 into diatom P, g P g P m^{-3} d^{-1}

$$UPPP2 = MIN(upo2, ppma * PRPC2) \quad (3.59)$$

GRPP2: Grazing of diatom P, g P m^{-3} d^{-1}

$$GRPP2 = pp2pc2 * GRPC2 \quad (3.60)$$

DEPP2: Death of diatom P, g P m^{-3} d^{-1}

$$DEPP2 = pp2pc2 * DEPC2 \quad (3.61)$$

SEPP2: Settling of diatom P, g P m^{-3} d^{-1}

$$SEPP2 = pp2pc2 * SEPC2 \quad (3.62)$$

Where:

Name	Comment	Unit	Type*)
pnma	Max. intracellular algae P	g P g C^{-1}	C
upo2	Potential PO_4 uptake by diatom	g P m^{-3} d^{-1}	A
pp2pc2	Diatom P:C ration	g P g C^{-1}	A
PC2	Diatom C	g C m^{-3}	S
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
SEPC2	Settling of diatom C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.9 PP3, Cyanobacteria P, g P m^{-3}

$$\frac{dPP3}{dt} = UPPP3 + UPLDOPP3 - GRPP3 - DEPP3 - SEPP3 - BUOYP3 \quad (3.63)$$

Where:

Process	Comment	Unit
UPPP3	Uptake of PO_4 into cyanobacteria P	g P m^{-3} d^{-1}
UPLDOPP3	Cyanobacteria uptake of LDOP	g P m^{-3} d^{-1}
GRPP3	Grazing of cyanobacteria P	g P m^{-3} d^{-1}
DEPP3	Death of cyanobacteria P	g P m^{-3} d^{-1}
SEPP3	Settling of cyanobacteria P	g P m^{-3} d^{-1}
BUOYP3	Upward movement cyanobacteria	g P m^{-3} d^{-1}

UPPP3: Uptake of PO_4 into cyanobacteria P, g P m^{-3} d^{-1}

$$UPPP3 = MIN(upo3, ppma * PRPC3) \quad (3.64)$$

UPLDOPP3: Cyanobacteria uptake of LDOP, g P m^{-3} d^{-1}

$$UPLDOPP3 = IF\ PO4 < 0.001\ THEN$$
$$IF\ \left(\left(ppma - \frac{PP3}{PC3}\right) < epsi, 0, maxupip * pda3 * 0.1 * \frac{LDOP}{(LDOP + hupp * pdb3 * 0.1)} * PC3\right) \quad (3.65)$$
$$ELSE\ 0$$

GRPP3: Grazing of cyanobacteria P, g P m^{-3} d^{-1}

$$GRPP3 = pp3pc3 * GRPC3 \quad (3.66)$$

DEPP3: Death of cyanobacteria P, g P m^{-3} d^{-1}

$$DEPP3 = pp3pc3 * DEPC3 \quad (3.67)$$

SEPP3: Settling of cyanobacteria P, g P m^{-3} d^{-1}

$$SEPP3 = pp3pc3 * SEPC3 \quad (3.68)$$

BUOYP3: Upward movement of PP3, g P m^{-3} d^{-1}

$$BUOYP3 = pp3pc3 * BUOYC3 \quad (3.69)$$

Where:

Name	Comment	Unit	Type*)
ppma	Max. intracellular algae P	g P g C^{-1}	C
upo3	Potential PO_4 uptake by cyanobacteria	g P m^{-3} d^{-1}	A
epsi	Small value	n.u.	C
maxupip	Max. PO_4 uptake by flagellates during P	g P g C^{-1}	C
LDOP	Labile DOP	g P m^{-3}	S
pda3	Ratio, nutrient uptake cyanobacteria:flagellates	n.u.	A
pdb3	Halfsaturation conc. Cyanobacteria:flagellates	n.u.	A
pp3pc3	Cyanobacteria P:C ratio	g P g C^{-1}	A
PC3	Cyanobacteria C	g C m^{-3}	S
PP3	Cyanobacteria P	g C m^{-3}	S
GRPC3	Grazing of cyanobacteria C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
SEPC3	Settling of cyanobacteria C	g C m^{-3} d^{-1}	P
BUOYC3	Upwared movement of cyanobacteria C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.10 PSi2, Diatom Si, g Si m^{-3}

$$\frac{dPSi2}{dt} = UPSi2 - GRPSi2 - DEPSi2 - SEPSi2 \quad (3.70)$$

Where:

Process	Comment	Unit
UPSi2	Uptake of Si into diatoms Si	g Si m^{-3} d^{-1}
GRPSi2	Grazing of diatoms Si	g Si m^{-3} d^{-1}
DEPSi2	Death of diatoms Si	g Si m^{-3} d^{-1}
SEPSi2	Settling of diatoms Si	g Si m^{-3} d^{-1}

UPSi2: Uptake of Si into diatom Si, g Si m^{-3} d^{-1}

$$UPSi2 = MIN(upsi, psma * PRPC2) \quad (3.71)$$

GRPSi2: Grazing of diatomSiP, g Si m^{-3} d^{-1}

$$GRPSi2 = psi2pc2 * GRPC2 \quad (3.72)$$

DEPSi2: Death of diatom Si, g Si m^{-3} d^{-1}

$$DEPSi2 = psi2pc2 * DEPC2 \quad (3.73)$$

SEPSi2: Settling of diatom Si, g Si m^{-3} d^{-1}

$$SEPSi2 = psi2pc2 * SEPC2 \quad (3.74)$$

Where:

Name	Comment	Unit	Type*)
psma	Max. intracellular algae Si	g Si g C $^{-1}$	C
usi2	potential Si uptake by diatom	g Si m^{-3} d^{-1}	A
psi2pc2	Diatom Si:C ration	Si P g C^{-1}	A
PC2	Diatom C	g C m^{-3}	S
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
SEPC2	Settling of diatom C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.11 CH, Chlorophyll, g m^{-3}

$$\frac{dCH}{dt} = PRCH - DECH - SECH - BUOYCH - GRCH \quad (3.75)$$

Where:

Process	Comment	Unit
PRCH	Net production phytoplankton chlorophyll	g Chl m^{-3} d^{-1}
SECH	Settling of phytoplankton chlorophyll	g Chl m^{-3} d^{-1}
DECH	Death of phytoplankton chlorophyll	g Chl m^{-3} d^{-1}
BUOYCH	Upward movement of CH	g Chl m^{-3} d^{-1}
GRCH	Zooplankton grazing on CH	g Chl m^{-3} d^{-1}

PRCH: Net production phytoplankton chlorophyll, g Chl m^{-3} d^{-1}

The production of chlorophyll

$$PRCH = PRPC1 * \frac{chmi}{ik1} * e^{chma*myn1} + PRPC2 * \frac{chmi}{ik2} * e^{chma*myn2} + PRPC3 * \frac{chmi}{ik1} * e^{chma*myn3} \quad (3.76)$$

SECH: Settling of phytoplankton chlorophyll, g Chl m^{-3} d^{-1}

$$SECH = \frac{CH}{PC1 + PC2 + PC3} * (SEPC1 + SEPC2 + SEPC3) \quad (3.77)$$

DECH: Death of phytoplankton chlorophyll, g Chl m^{-3} d^{-1}

$$DECH = \frac{CH}{PC1 + PC2 + PC3} * (DEPC1 + DEPC2 + DEPC3) \quad (3.78)$$

GRCH: ZC Grazing on CH, g Chl m^{-3} d^{-1}

$$GRCH = \frac{CH}{PC1 + PC2 + PC3} * (GRPC1 + GRPC2 + GRPC3) \quad (3.79)$$

Where:

Name	Comment	Unit	Type*)
PC1	Flagellate C	g C m^{-3}	S
PC2	Diatom C	g C m^{-3}	S
PC3	Cyanobacteria C	g C m^{-3}	S
chmi	Min. chlorophyll-a production	mol photon$^{-1}m^{-2}d^{-1}$	C
chma	Max. chlorophyll-a producti	mol photon$^{-1}m^{-2}d^{-1}$	C
myn1	Nitrogen function Flagellate	n.u.	A
myn2	Nitrogen function Diatom	n.u.	A
myn2	Nitrogen function Cyanobacteria	n.u.	A
ik1	Light saturation temp. corrected, PC1, PC3	mol photon $m^{-2}d^{-1}$	A
Ik2	Light saturation temp. corrected, PC2	mol photon $m^{-2}d^{-1}$	A
PRPC1	Net production of flagellate C	g C m^{-3} d^{-1}	P
SEPC1	Sedimentation of flagellate C	g C m^{-3} d^{-1}	P
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
GRPC1	Grazing of flagellate C	g C m^{-3} d^{-1}	P
PRPC2	Net production of diatom C	g C m^{-3} d^{-1}	P
SEPC2	Sedimentation of diatom C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
PRPC3	Net production of cyanobacteria C	g C m^{-3} d^{-1}	P
SEPC3	Sedimentation of cyanobacteria C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
GRPC3	Grazing of cyanobacteria C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.12 ZC, zooplankton, g C m^{-3}

$$\frac{dZC}{dt} = PRZC - DEZC \tag{3.80}$$

Where:

Process	Comment	Unit
PRZC	Net production of zooplankton carbon	g C m^{-3} d^{-1}
DEZC	Death of zooplankton carbon	g C m^{-3} d^{-1}

PRZC: Production of zooplankton carbon, g C m^{-3} d^{-1}

$$PRZC = vefo * (GRPC1 + GRPC2 + GRPC3) \tag{3.81}$$

DEZC: Death of zooplankton carbon, g C m^{-3} d^{-1}

$$DEZC = kdz * zc^2 + kdzb * zc \tag{3.82}$$

Where:

Name	Comment	Unit	Type*)
vefo	Zooplankton growth efficiency	g C g C^{-1}	C
kdz	Zooplankton death rate 2nd order,	m^3 (g C*d)$^{-1}$	C
kdzb	Zooplankton death rate 1st order	d^{-1}	C
GRPC1	Grazing of flagellate C	g C m^{-3} d^{-1}	P
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
GRPC3	Grazing of cyanobacteria C	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.13 DC, Detritus C, g C m^{-3}

$$\frac{dDC}{dt} = EKZC + DEZC + DEPC2DC - REDC - deDCw - SREDC - SEDC \quad (3.83)$$

Where:

Process	Comment	Unit
EKZC	Excretion by zooplankton carbon	g C m^{-3} d^{-1}
DEZC	Death of zooplankton carbon	g C m^{-3} d^{-1}
DEPC2DC	Death phytoplankton to detritus carbon	g C m^{-3} d^{-1}
REDC	DO mineralisation of detritus carbon	g C m^{-3} d^{-1}
deDCw	DC anaerobic respiration with NO_3	g C m^{-3} d^{-1}
SREDC	DC anaerobic oxidation with SO_4	g C m^{-3} d^{-1}
SEDC	Settling of detritus carbon	g C m^{-3} d^{-1}

EKZC: Excretion by zooplankton carbon, g C m^{-3} d^{-1}

$$EKZC = (1 - vefo - refo) * (GRPC1 + GRPC2 + GRPC3) \quad (3.84)$$

DEZC: Death of zooplankton carbon, g C m^{-3} d^{-1}

DEZC: see processes for zooplankton C, ZC, Equation (3.82)

DEPC2DC: Death phytoplankton to detritus carbon, g C m^{-3} d^{-1}

$$DEPC2DC = (1 - vm - vp - vn) * (DEPC1 + DEPC2 + DEPC3) \quad (3.85)$$

REDC: DO mineralisation of detritus carbon, g C m^{-3} d^{-1}

$$EDC = kmdm * DC * tere^{T-20} * \frac{DO^{ndo2}}{MAX(0.01, DO^{ndo2} + mdo2)} \quad (3.86)$$

deDCw: DC respiration with NO_3, g C m^{-3} d^{-1}

$$deDCw = (DENW * vn3 + ANAMOX * 0.429) * \frac{DC}{DC + LDOC} \quad (3.87)$$

SREDC: DC oxidation with SO_4, g C m^{-3} d^{-1}

$$sredc = SRED * vso * \frac{dc}{dc + LDOC} \tag{3.88}$$

SEDC: Settling of detritus carbon, g C m^{-3} d^{-1}

$$SEDC = ksd * \frac{dc}{dz} \tag{3.89}$$

Where:

Name	Comment	Unit	Type*)
vefo	Zooplankton growth effency	g C g C^{-1}	C
refo	Zooplankton, respiration	g C g C^{-1}	C
GRPC1	Grazing of flagellate C	g C m^{-3} d^{-1}	P
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
GRPC3	Grazing of cyanobacteria C	g C m^{-3} d^{-1}	P
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
vm	Fraction of PC mineralised at PC death	n.u.	C
vp	Fraction of PC to CDOC-N&P at PC death	n.u.	C
vn	Fraction of PC to LDOC-N&P at PC death	n.u.	C
kmdm	DC mineralisation rate at 20 ° C	d^{-1}	C
tere	Θ in Arrhenius function, DC mineralisation	n.u.	C
T	Temperature	°C	F
DO	Oxygen	g O_2 m^{-3}	S
ndo2	DC & LDOC:Coefficient, DO mineralisation	n.u.	C
mdo2	DO half-saturation constant, DC & LDOC mineralisation	n.u	C
DENW	Denitrificaion in water using DC+LDOC	g N m^{-3} d^{-1}	P
vn3	C:N ratio denitrification	g C g N^{-1}	C
ANAMOX	Anammox, NO_3+NH_4 → N_2	g N m^{-3} d^{-1}	P

Name	Comment	Unit	Type*)
LDOC	Labile DOC	g C m^{-3}	S
SRED	SO_4 Respiration of DC+LDOC	g S m^{-3} d^{-1}	P
vso	C:S ratio C mineralisation SO_4 to H_2S	g C g S^{-1}	C
ksd	Sedimentation rate detritus	m d^{-1}	A
dz	Height of actual water layer in model	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.14 DN, Detritus N, g N m^{-3}

$$\frac{dDN}{dt} = EKZN + DEZN + DEPN2DN - REDN - SREDN - deDNw - SEDN \quad (3.90)$$

Where:

Process	Comment	Unit
EKZN	Excretion by zooplankton N	g N m^{-3} d^{-1}
DEZN	Death of zooplankton N	g N m^{-3} d^{-1}
DEPN2DN	Death phytoplankton to detritus N	g N m^{-3} d^{-1}
REDN	DO mineralisation of detritus N to NH_4	g N m^{-3} d^{-1}
deDNw	Anaerobic respiration of DN with NO_3 to NH_4	g N m^{-3} d^{-1}
SREDN	Anaerobic oxidation of DN with SO_4 to NH_4	g N m^{-3} d^{-1}
SEDN	Settling of detritus N	g N m^{-3} d^{-1}

EKZN: Excretion by zooplankton N, g N m^{-3} d^{-1}

$$EKZN = (1 - vefo - refo) * (GRPN1 + GRPN2 + GRPN3) \quad (3.91)$$

DEZN Death of zooplankton N, g N m^{-3} d^{-1}

$$DEZN = vzn * DEZC \quad (3.92)$$

DEPN2DN: Death phytoplankton to detritus N, g N m^{-3} d^{-1}

$$DEPN2DN = (1 - vm - vp - vn) * (DEPN1 + DEPN2 + DEPN3) \quad (3.93)$$

REDN: DO mineralisation of detritus N, g N m^{-3} d^{-1}

$$REDN = kmdn * dndc * REDC \quad (3.94)$$

deDNw: DN respiration with NO3, g N m^{-3} d^{-1}

$$deDNw = deDCw * dndc \quad (3.95)$$

SREDN: DN oxidation with SO4, g N m^{-3} d^{-1}

$$SREDN = SREDC * dndc \quad (3.96)$$

SEDN: Settling of detritus N, g N m^{-3} d^{-1}

$$SEDN = SEDC * dndc \quad (3.97)$$

Where:

Name	Comment	Unit	Type*)
vefo	Zooplankton growth effency	g C g C^{-1}	C
refo	Zooplankton, respiration	g C g C^{-1}	C
GRPN1	Grazing of flagellate N	g N m^{-3} d^{-1}	P
GRPN2	Grazing of diatom N	g N m^{-3} d^{-1}	P
GRPN3	Grazing of cyanobacteria N	g N m^{-3} d^{-1}	P
DEPN1	Death of flagellate N	g N m^{-3} d^{-1}	P
DEPN2	Death of diatom N	g N m^{-3} d^{-1}	P
DEPN3	Death of cyanobacteria N	g N m^{-3} d^{-1}	P
vzn	N:C ratio Zooplankton	g N g C^{-1}	C
vm	Fraction of PC mineralised at PC death	n.u.	C
vp	Fraction of PC to CDOC-N&P at PC death	n.u.	C
vn	Fraction of PC to LDOC-N&P at PC death	n.u.	C
kmdn	Factor N mineralisation of DN	n.u.	C
dndc	N:C ration, detritus	g N g C^{-1}	A
REDC	DO mineralisation of detritus carbon	g C m^{-3} d^{-1}	P

Name	Comment	Unit	Type*)
deDCw	Anaerobic DC respiration with NO_3	g C m^{-3} d^{-1}	P
SREDC	Anaerobic DC oxidation with SO_4	g C m^{-3} d^{-1}	P
SEDC	Settling of detritus carbon	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.15 DP, Detritus P, g P m^{-3}

$$\frac{dDP}{dt} = EKZP + DEZP + DEPP2DP - REDP - SREDP - deDPw - SEDP \quad (3.98)$$

Where:

Process	Comment	Unit
EKZP	Excretion by zooplankton P	g P m^{-3} d^{-1}
DEZP	Death of zooplankton P	g P m^{-3} d^{-1}
DEPP2DNP	Death phytoplankton to detritus P	g P m^{-3} d^{-1}
REDP	DO mineralisation of detritus P to PO_4	g P m^{-3} d^{-1}
deDPw	Anaerobic respiration of DP with NO_3 to PO_4	g P m^{-3} d^{-1}
SREDP	Anaerobic oxidation of DP with SO_4 to PO_4	g P m^{-3} d^{-1}
SEDP	Settling of detritus P	g P m^{-3} d^{-1}

EKZP: Excretion by zooplankton P, g P m^{-3} d^{-1}

$$EKZP = (1 - vefo - refo) * (GRPP1 + GRPP2 + GRPP3) \quad (3.99)$$

DEZP: Death of zooplankton P, g P m^{-3} d^{-1}

$$DEZP = vzp * DEZC \quad (3.100)$$

DEPP2DP: Death phytoplankton to detritus P, g P m^{-3} d^{-1}

$$DEPP2DP = (1 - vm - vp - vn) * (DEPP1 + DEPP2 + DEPP3) \quad (3.101)$$

REDP: DO mineralisation of detritus P, g P m^{-3} d^{-1}

$$REDP = kmdp * dpdc * REDC \quad (3.102)$$

deDPw: DP respiration with NO_3, g P m^{-3} d^{-1}

$$deDPw = deDCw * dpdc \quad (3.103)$$

SREDP: DP oxidation with SO_4, g P m^{-3} d^{-1}

$$SREDP = SREDC * dpdc \quad (3.104)$$

SEDP: Settling of detritus P, g P m^{-3} d^{-1}

$$SEDP = SEDC * dpdc \quad (3.105)$$

Where:

Name	Comment	Unit	Type*)
vefo	Zooplankton growth effency	g C g C^{-1}	C
refo	Zooplankton, respiration	g C g C^{-1}	C
GRPP1	Grazing of flagellate P	g P m^{-3} d^{-1}	P
GRPP2	Grazing of diatom P	g P m^{-3} d^{-1}	P
GRPP3	Grazing of cyanobacteria P	g P m^{-3} d^{-1}	P
DEPP1	Death of flagellate P	g P m^{-3} d^{-1}	P
DEPP2	Death of diatom P	g P m^{-3} d^{-1}	P
DEPP3	Death of cyanobacteria P	g P m^{-3} d^{-1}	P
vzp	P:C ratio Zooplankton	g P g C^{-1}	C
vm	Fraction of PC mineralised at PC death	n.u.	C
vp	Fraction of PC to CDOC-N&P at PC death	n.u.	C
vn	Fraction of PC to LDOC-N&P at PC death	n.u.	C
kmdp	Factor P mineralisation of DP	n.u.	C
dpdc	P:C ration, detritus	g P g C^{-1}	A
REDC	DO mineralisation of detritus carbon	g C m^{-3} d^{-1}	P
deDCw	Anaerobic DC respiration with NO_3	g C m^{-3} d^{-1}	P

Name	Comment	Unit	Type*)
SREDC	Anaerobic DC oxidation with SO_4	g C m^{-3} d^{-1}	P
SEDC	Settling of detritus carbon	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.16 DSi, Detritus Si, g Si m^{-3}

$$\frac{dDSi}{dt} = DEPSi2 + GRPSi2 - REDSi - SEDSi \quad (3.106)$$

Where:

Process	Comment	Unit
DEPSi2	Death phytoplankton Si to detritus Si	g Si m^{-3} d^{-1}
GRPSi2	Grazing of Diatom Si	g Si m^{-3} d^{-1}
REDSi	DO mineralisation of detritus Si to Si	g Si m^{-3} d^{-1}
SEDSi	Settling of detritus Si	g Si m^{-3} d^{-1}

DEPSi2: Death phytoplankton Si to detritus Si, g Si m^{-3} d^{-1}

$$DEPSi2 = DEPC2 * psi2pc2 \quad (3.107)$$

GRPSi2: Grazing of Diatom Si, g Si m^{-3} d^{-1}

$$GRSi2 = GRPC2 * psi2pc2 \quad (3.108)$$

REDSi: DO mineralisation of detritus Si to Si, g Si m^{-3} d^{-1}

$$REDSi = REDC * dsidc * kmds \quad (3.109)$$

SEDSi: Settling of detritus Si, g Si m^{-3} d^{-1}

$$SEDSi = SEDC * dsidc \quad (3.110)$$

Where:

Name	Comment	Unit	Type*)
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
psi2pc2	Si:C ration, Diatom	g Si g C^{-1}	A
GRPC2	Grazing of diatom C	g C m^{-3} d^{-1}	P
REDC	DO mineralisation of detritus carbon	g C m^{-3} d^{-1}	P
dsidc	Si:C ration, detritus	g Si g C^{-1}	A
kmds	Factor Si mineralisation of DSi	n.u.	C
SEDC	Settling of detritus carbon	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.17 NH4, Total ammonia, g N m^{-3}

$$\frac{dNH4}{dt} = REDN + REZN + deDNw + SREDN + reLDON + deLDON + sreLDON + feunh4m3 + fsnb + NH4dep + DEPN2NH - RNIT - ANAMOX - UPNH1 - UPNH2 - UPNH3 \quad (3.111)$$

Where:

Process	Comment	Unit
REDN	DN→NH_4 via DO oxidation of DC	g N m^{-3} d^{-1}
REZN	Respiration of zooplankton nitrogen	g N m^{-3} d^{-1}
deDNw	DN→NH_4 denitrification mineralisation of DC	g N m^{-3} d^{-1}
SREDN	DN →NH_4 via SO_4 mineralisation of DC	g N m^{-3} d^{-1}
reLDON	LDON→NH_4 via DO oxidation of LDOC	g N m^{-3} d^{-1}
deLDON	LDON →NH_4 via denitrification mineralisation of LDOC	g N m^{-3} d^{-1}
sreLDON	LDON →NH_4 via SO_4 mineralisation of LDOC	g N m^{-3} d^{-1}
feunh4m3	NH_4 flux between sediment pore water and water	g N m^{-3} d^{-1}
fsnb	Mineralisation of newly settled organic N	g N m^{-3} d^{-1}
NH4dep	Atmospheric NH_4 deposition	g N m^{-3} d^{-1}
DEPN2NH	Fraction of DEPN1-3 to NH_4	g N m^{-3} d^{-1}

Process	Comment	Unit
RNIT	Nitrification in water column	g N m^{-3} d^{-1}
ANAMOX	Anammox, NO_3+NH_4 → N_2	g NH_4-N m^{-3} d^{-1}
UPNH1	NH_4 uptake by flagellate	g N m^{-3} d^{-1}
UPNH2	NH_4 uptake by diatom	g N m^{-3} d^{-1}
UPNH3	NH_4 uptake by cyanobacteria	g N m^{-3} d^{-1}

REDN: NH4 production via mineralisation of DC, DN & DP with DO, g N m^{-3} d^{-1}

Please see under DN, Equation (3.94)

REZN: Respiration of zooplankton nitrogen, g N m^{-3} d^{-1}

$$REZN = (\mathrm{GRPN1} + \mathrm{GRPN2} + \mathrm{GRPN3}) * vzn - EKZN \quad (3.112)$$

Where: **EKZN: Excretion of N by zooplankton**

$$EKZN = (1 - \mathrm{vefo} - \mathrm{refo}) * (\mathrm{GRPN1} + \mathrm{GRPN2} + \mathrm{GRPN3}) \quad (3.113)$$

deDNw: NH4 production via denitrificatiation (NO3 mineralisation) of DC, DN & DP, g N m^{-3} d^{-1}

Pease see under DN, Equation (3.95)

SREDN: NH4 production via anaerobic SO4 mineralisation of DC, DN & DP, g N m^{-3} d^{-1}
Please see under DN, Equation (3.96)

reLDON: NH4 production via mineralisation of LDOC, LDON & LDOP with DO, g N m^{-3} d^{-1}
Please see under LDON (Section 3.3.27).

deLDON: NH4 production via denitrificatiation, (mineralisation) of LDOC, LDON & LDOP, g N m^{-3} d^{-1}

Please see under LDON (Section 3.3.27).

sreLDON: NH4 production via anaerobic SO4 mineralisation of LDOC, LDON & LDOP, g N m^{-3} d^{-1}

Please see under LDON (Section 3.3.27).

feunh4m3: NH4 flux between sediment pore water and water, g N m^{-3} d^{-1}

$$feunh4m3 = feunh4/dz \tag{3.114}$$

fsnb: Mineralisation of newly settled organic N, g N m^{-3} d^{-1}

$$fsnb = krsn0 * (SEPN1 - BUOYN1 + SEPN2 + SEPN3 - BUOYN3 + SEDN - depoC * knim/dz) * tetn^{T-20} \tag{3.115}$$

NH4dep: Atmospheric N deposition as NH4 to surface layer, g N m^{-3} d^{-1}

$$NH4depo = NHdep/dz \tag{3.116}$$

RNIT: Nitrification in water column, g N m^{-3} d^{-1}

$$RNIT = \text{knitw} * tnit^{T-20} * \text{sqdo} * \frac{NH4}{NH4 + hmt} * \text{NH4} \tag{3.117}$$

ANAMOX: Anammox, NO3+NH4 → N2, , g NH4-N m^{-3} d^{-1}

$$ANAMOX = IF\ DO < 0.32\ THEN$$

$$kanam * tetn^{T-20} * \frac{NH4}{NH4 + hun4} * \frac{NO3}{NO3 + hun3} * \frac{DC + LDOC}{DC + LDOC + hudc1} \tag{3.118}$$

$$ELSE\ 0$$

UPNH1-3: NH4 uptake by phytoplankton, g N m^{-3} d^{-1}

UPNH1, UPNH2 & UPNH3 see under PN1 (Section 3.3.4), PN2 (Section 3.3.5) and PN3 (Section 3.3.6)

Where:

Name	Comment	Unit	Type*)
vzn	N to C ratio in zooplankton,	g N g C^{-1}	C
GRPN1	Grazing of flagellate N	g N m^{-3} d^{-1}	P
GRPN2	Grazing of diatom N	g N m^{-3} d^{-1}	P
GRPN3	Grazing of cyanobacteria N	g N m^{-3} d^{-1}	P
EKZN	Excretion of N by zooplankton	g N m^{-3} d^{-1}	P
vefo	Zooplankton growth effency	g C g C^{-1}	C

Name	Comment	Unit	Type*)
refo	Zooplankton, respiration	g C g C^{-1}	C
feunh4	Flux of NH_4 from sediment to water	g N m^{-2} d^{-1}	P
SEPN1	Settling of flagellate N	g N m^{-3} d^{-1}	P
SEPN2	Settling of diatom N	g N m^{-3} d^{-1}	P
SEPN3	Settling of cyanobacteria N	g N m^{-3} d^{-1}	P
BUOYN1	Upward movement of flagellate N	g N m^{-3} d^{-1}	P
BUOYN3	Upward movement of cyanobacteria N	g N m^{-3} d^{-1}	P
depoC	Deposition of organic C to sediment	g C m^{-2} d^{-1}	P
knim	Sediment: N:C ratio of immobile N	g N g C^{-1}	C
tetn	Θ value in Arrhenius equation for N	n.u.	C
T	Temperature Deg. Celsius	°C	C
NHdep	Atmospheric N deposition	g N m^{-2} d^{-1}	F
knitw	Specific nitrification water at 20 C	d^{-1}	C
tnit	Θ value in Arrhenius equation for nitrification	n.u.	C
hmt	Halfsaturation NH_4 nitrification	g N m^{-3} d^{-1}	C
sqdo	DO function	n.u.	A
kanam	max anammox NO_3-N or NH_4-N concumption	g N m^{-3} d^{-1}	C
NO3	NO_3 –N	g N m^{-3}	S
hun4	NH_4 half satutation conc., anammox & thiodenitrification	g N m^{-3}	C
hun3	NO_3 half saturation concentration, anammox	g N m^{-3}	C
DC	Detrituc C	g C m^{-3}	S
LDOC	Labile DOC	g C m^{-3}	S
hudc1	DC+LDC Half saturation concentration, anammox	g C m^{-3}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.18 NO3, Nitrate, g N m^{-3}

$$\frac{dNO3}{dt} = RNIT + feuno3m3 + NO3dep - DENW - DENW_S - ANAMOX - UPN31 - UPN32 - UPN33 \quad (3.119)$$

Where:

Process	Comment	Unit
RNIT	Nitrification in water column	g N m^{-3} d^{-1}
feuno3m3	Flux of NO_3 between water & sediment	g N m^{-3} d^{-1}
NO3dep	Atmospheric deposition of NO_3 at the water surface	g N m^{-3} d^{-1}
DENW	Denirification water	g N m^{-3} d^{-1}
$DENW_s$	Thiodenitification, $4NO_3+3H_2S \rightarrow 2N_2+3SO_4$	g N m^{-3} d^{-1}
ANAMOX	Anammox, $NO_3+NH_4 \rightarrow N_2$	g NO_3-N m^{-3} d^{-1}
UPN31	NO_3 uptake by flagellate	g N m^{-3} d^{-1}
UPN32	NO_3 uptake by diatom	g N m^{-3} d^{-1}
UPN32	NO_3 uptake by cyanobacteria	g N m^{-3} d^{-1}

RNIT: Nitrification in water column, g N m^{-3} d^{-1}

Please see under NH4, Equation (3.117)

feuno3m3: Flux of NO3 between water & sediment, g N m^{-3} d^{-1}

$$feuno3m3 = feuno3/dz \quad (3.120)$$

NO3dep: Atmospheric deposition of NO3 at the water surface, g N m^{-3} d^{-1}

$$NO3dep = NO3depo/dz \quad (3.121)$$

DENW: Denirification water, g N m^{-3} d^{-1}

$denw =$ IF $DO <$ mdo3 THEN

$$kdenw * tetn^{T-20} * \frac{ksb + 0.1}{DO + ksb + 0.1} * \frac{N03}{NO3 + hun3} * \frac{DC + LDOC}{DC + LDOC + hudc} \quad (3.122)$$

ELSE 0

DENWS: Thiodenitification, 4NO3+3H2S→2N2+3SO4, g N m^{-3} d^{-1}

$$DENW_s = IF\ DO < 0.32\ THEN$$

$$kdenw * tetn^{T-20} * \frac{H2S}{H2S + hs1} * \frac{NO3}{NO3 + hun3} * \frac{hudc}{DC + LDOC + hudc} \quad (3.123)$$

$$ELSE\ 0$$

ANAMOX: Anammox, NO3+NH4 → N2 , g NO3-N m^{-3} d^{-1}

$$ANAMOX = IF\ DO < 0.32\ THEN$$

$$kanam * tetn^{T-20} * \frac{NH4}{NH4 + hun4} * \frac{NO3}{NO3 + hun3} * \frac{DC + LDOC}{DC + LDOC + hudc1} \quad (3.124)$$

$$ELSE\ 0$$

UPN31, UPN32, UPN33: NO3 uptake flagellates, diatoms and cyanobacteria, g N m^{-3} d^{-1}

Please see under PN1 (Section 3.3.4), PN2 (Section 3.3.5) and PN3 (Section 3.3.6)

Where:

Name	Comment	Unit	Type*)
feuno3	Nitrate flux between sediment and water column	g N m^{-2} d^{-1}	P
NO3depo	Atmospheric NO_3-N deposition to water surface	g N m^{-2} d^{-1}	F
mdo3	DO limit for denitrification in water column & half saturation concentration in sqdo	g O_2 m^{-3}	C
Kdenw	Max. denitrification at 20 °C in water column	g N m^{-3} d^{-1}	C
ksb	Half saturation DO conc. for denitrification	g O_2 m^{-3}	C
tetn	Θ in Arrhenius function, denitrifications temperature dependency	n.u	C
hun3	NO_3 half saturation concentration for denitrification	g N m^{-3}	C
hudc	DC+LDOC Half saturation concentration for SO_4 reduction & denitrification	g C m^{-3}	C
DC	Detritus C	g C m^{-3}	S
LDOC	Labile fraction of DOC	g C m^{-3}	S
tetn	Θ value in Arrhenius equation for N	n.u.	C

Name	Comment	Unit	Type*)
T	Temperature	°C	F
H2S	H_2S-S	g S m^{-3}	S
hs1	H2S half saturation thiodenitirfication	g S m^{-3}	C
NH4	NH_4-N	g N m^{-3}	S
hun4	NH_4 half satutation conc., anammox & thiodenitrification	g N m^{-3}	C
hudc1	DC+LDC Half saturation concentration, anammox	g C m^{-3}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.19 H2S, Hydrogen Sulphide, g S m^{-3}

$$\frac{dH2S}{dt} = SRED + fwsh2sm3 - SOXI - SOXI_N \quad (3.125)$$

Where:

Process	Comment	Unit
SRED	Anaerobic SO_4 Respiration of DC+LDOC	g S m^{-3} d^{-1}
fwsh2sm3	H_2S flux from sediment to water	g S m^{-3} d^{-1}
SOXI	Oxidation of H_2S	g S m^{-3} d^{-1}
$SOXI_N$	SO_4 production by thiodenitrification, $4NO_3+3H_2S \rightarrow 2N_2+3SO_4$	g S m^{-3} d^{-1}

SRED: SO_4 Respiration of DC+LDOC, g S m^{-3} d^{-1}

$$SRED = IF\ DO < 0.5\ THEN$$

$$ksc * fsa * ts4r^{(T-20)} * \frac{hun3}{NO3 + hun3} * \frac{DC + LDOC}{DC + LDOC + hudc} \quad (3.126)$$

$$ELSE\ 0$$

fwsh2sm3: H_2S flux from sediment to water, g S m^{-3} d^{-1}

$$fwsh2sm3 = fwh2s/dz \quad (3.127)$$

SOXI: Oxidation of H_2S, g S m^{-3} d^{-1}

$$SOXI = kse * ksf^{(T-20)} * H2S * sqdo \quad (3.128)$$

$SOXI_N$: SO_4 production by thiodenitrification, $4NO_3+3H_2S-->2N_2+3SO_4$, g S m^{-3} d^{-1}

$$SOXI_N = DENW_S * 1.429 \quad (3.129)$$

Where:

Name	Comment	Unit	Type*)
Ksc	Max. anoxic DC +LDOC respiration rate with SO_4	g S m^{-3} d^{-1}	C
Fsa	Salinity function for reduction of SO4 to H2S	n.u.	A
hun3	NO_3 half saturation concentration for denitrification	g N m^{-3}	C
Hudc	DC+LDOC Half saturation concentration for SO_4 reduction & denitrification	g C m^{-3}	C
DC	Detritus C	g C m^{-3}	S
LDOC	Labile fraction of DOC	g C m^{-3}	S
ts4r	Θ value in Arrhenius function for SO_4 reductions temperature dependency.	n.u.	C
fwh2s	Flux of reduced H_2S equialents from sediment to water	g S $m^{-2}d^{-1}$	P
Kse	Max. specific oxidation rate of H2S, 20 deg. °C	d^{-1}	C
Ksf	Θ value in Arrhenius function for SO_4 oxidations temperature dependency.	n.u.	C
Sqdo	DO function	n.u.	A
$DENW_S$	Thiodenitification. $4NO_3+3H_2S→2N_2+3SO_4$	g N $m^{-3}d^{-1}$	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.20 IP, Phosphate (PO4-P), g P m^{-3}

$$\frac{dIP}{dt} = REDP + REZP + reLDOP + deLDOP + sreLDOP + deDPw + SREDP + DEPP2IP + fspb + fsipm3 + Pdep - UPPP1 - UPPP2 - UPPP3 \quad (3.130)$$

Where:

Process	Comment	Unit
REDP	DP→PO_4 via DO oxidation of DC	g P m^{-3} d^{-1}
REZP	Respiration of zooplankton P	g P m^{-3} d^{-1}
reLDOP	LDOP→PO_4 via DO oxidation of LDOC	g P m^{-3} d^{-1}
deLDOP	LDOP →PO_4 via denitrification mineralisation of LDOC	g P m^{-3} d^{-1}
sreLDOP	LDOP →PO_4 via SO_4 mineralisation of LDOC	g P m^{-3} d^{-1}
deDPw	DP→PO_4 denitrification mineralisation of DC	g P m^{-3} d^{-1}
SREDP	DP →PO_4 via SO_4 mineralisation of DC	g P m^{-3} d^{-1}
DEPP2IP	Dead Plankton P to PO_4	g P m^{-3} d^{-1}
fspb	Mineralisation of newly settled organic P	g P m^{-3} d^{-1}
fsipm3	PO_4 flux between sediment pore water and water	g P m^{-3} d^{-1}
Pdep	Atmospheric P deposition	g P m^{-3} d^{-1}
UPPP1	PO_4 uptake by flagellates	g P m^{-3} d^{-1}
UPPP2	PO_4 uptake by Diatoms	g P m^{-3} d^{-1}
UPPP3	PO_4 uptake by cyanobacteria	g P m^{-3} d^{-1}

REDP: PO_4 production via mineralisation of DC, DN & DP with DO, g P m^{-3} d^{-1}

Please see under state variable DP, Section 3.3.15

REZP: Respiration of zooplankton phosphorus, g P m^{-3} d^{-1}

$$REZP = \mathrm{MAX}(0, \mathrm{GRPP1} + \mathrm{GRPP2} + \mathrm{GRPP3} - \mathrm{PRZC} * vzp - EKZP) \quad (3.131)$$

reLDOP: PO4 production via mineralisation of LDOC, LDON & LDOP with DO, g P m^{-3} d^{-1}

$$reLDOP = \frac{LDOP}{LDOC} * reLDOC \quad (3.132)$$

deLDOP: PO4 production via denitrificatiation (mineralisation) of LDOC, LDON & LDOP, g P m^{-3} d^{-1}

$$deLDOP = \frac{LDOP}{LDOC} * deLDOC \tag{3.133}$$

sreLDOP: PO4 production via anaerobic SO4 mineralisation of LDOC, LDON & LDOP, g P m^{-3} d^{-1}

$$sreLDOP = \frac{LDOP}{LDOC} * sreLDOC \tag{3.134}$$

deDPw: PO4 production via anaerobic denitrificatiation (mineralisation) of DC, DN & DP, g P m^{-3} d^{-1}

Please see under DP, Section 3.3.15

SREDP: PO4 production via anaerobic SO4 mineralisation of DC, DN & DP, g P m^{-3} d^{-1}

Please see under DP, Section 3.3.15

DEPP2IP: Dead Plankton P to PO4 , g P m^{-3} d^{-1}

$$\mathrm{DEPP2IP} = (\mathrm{DEPP1} + \mathrm{DEPP2} + \mathrm{DEPP3}) * \mathrm{vm} \tag{3.135}$$

fspb: Mineralisation of newly settled organic P, g P m^{-3} d^{-1}

$$fspb = krsp0 * (SEPP1 - BUOYP1 + SEPP2 + SEPP3 - BUOYP3 + SEDP) * tetp^{T-20} \tag{3.136}$$

fsipm3: PO4 flux between sediment pore water and water, g P m^{-3} d^{-1}

$$fsipm3 = fsip/dz \tag{3.137}$$

Pdep: Atmospheric P deposition as PO4 to surface layer, g P m^{-3} d^{-1}

$$Pdep = Pdepo/dz \tag{3.138}$$

UPPP1-3: PO4 uptake by flagellates, diatoms and cyanobacteria, g P m^{-3} d^{-1}

Please see under PP1 (Section 3.3.7), PP2 (Section 3.3.8), and PP3 (Section 3.3.9)

Where:

Name	Comment	Unit	Type*)
GRPP1	Grazing of phytoplankton (Flagellate) P	g P m^{-3} d^{-1}	P
GRPP2	Grazing of phytoplankton (diatom) P	g P m^{-3} d^{-1}	P
GRPP3	Grazing of cyanobacteria P	g P m^{-3} d^{-1}	P
PRZC	Net production of zooplankton C	g C m^{-3} d^{-1}	P
vzp	P:C ratio in zooplankton	g P g C^{-1}	C
EKZP	Excretion by zooplankton P	g P m^{-3} d^{-1}	P
reLDOC	DO respiration LDOC	g C m^{-3} d^{-1}	P
LDOP	Labile DOP	g P m^{-3}	S
LDOC	Labile DOC	g C m^{-3}	S
deLDOC	Anaerobic mineralisation of LDOC via denitrification	g C m^{-3} d^{-1}	P
sreLDOC	Anaerobic mineralisation of LDOC via SO_4 reduction	g C m^{-3} d^{-1}	P
DEPP1	Death of flagellate P	g P m^{-3} d^{-1}	P
DEPP2	Death of diatom P	g P m^{-3} d^{-1}	P
DEPP3	Death of cyanobacteria P	g P m^{-3} d^{-1}	P
vm	Fraction of PC mineralised at PC death	n.u.	C
krsp0	Fraction of newly settled P to mineralisation	n.u.	C
SEPP1	Sedimentation of flagellates P	g P m^{-3} d^{-1}	P
SEPP2	Sedimentation of diatom P	g P m^{-3} d^{-1}	P
SEPP3	Sedimentation of cyanobacteria P	g P m^{-3} d^{-1}	P
BUOYP1	Upward movement of flagellates P	g P m^{-3} d^{-1}	P
BUOYP3	Upward movement of cyanobacteria P	g P m^{-3} d^{-1}	P
SEDP	Sedimentation detritus P	g P m^{-3} d^{-1}	P
tetp	Θ value in Arrhenius equation for P	n.u.	C
T	Temperature Deg. Celsius	°C	C
fsip	PO_4 flux between pore water and water	g P m^{-2} d^{-1}	P
Pdep	Atmospheric P deposition	g P m^{-2} d^{-1}	F
dz	Height of actual water layer in model	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.21 IP, Phosphate (PO4-P), g P m^{-3}

$$\frac{dSi}{dt} = REDSi + RSSi2Si - UPSi2 \quad (3.139)$$

Where:

Process	Comment	Unit
REDSi	DO mineralisation of detritus DSi to Si	g Si $m^{-3}d^{-1}$
RSSi2Si	Si release fom sediment	g Si $m^{-3}d^{-1}$
UPSi2	Uptake of Si into diatom Si	g Si $m^{-3}d^{-1}$

DEPSi2: Death phytoplankton Si to detritus Si, g Si m^{-3} d^{-1}

Please see under DSi, Section 3.3.16

RSSi2Si: Si release fom sediment, g Si m^{-3} d^{-1}

$$RSSi2Si = RSSi/dz \quad (3.140)$$

UPSi2: Uptake of Si into diatom Si, g Si Si m^{-3} d^{-1}

Please see under Psi2, Section 3.3.10

Where:

Name	Comment	Unit	Type*)
RSSi	Si release form sediment	g Si m^{-2} d^{-1}	P
dz	Height of actual water layer in model	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.22 DO, Oxygen, g O2 m^{-3}

$$\frac{dDO}{dt} = ODPC + REAR + REAR1 - ODDC - ODZC - SOXI2DO - RNIT2DO - reLDOC2DO - DEPC2DO - ODSC \quad (3.141)$$

Where:

Process	Comment	Unit
ODPC	Net O_2 production by phytoplankton	g O_2 m^{-3} d^{-1}
REAR	Reaeration	g O_2 m^{-3} d^{-1}
REAR1	Reaeration shallow water	g O_2 m^{-3} d^{-1}
ODDC	DO consumption by mineralisation of DC	g O_2 m^{-3} d^{-1}
ODZC	Zooplankton respiration	g O_2 m^{-3} d^{-1}
SOXI2DO	DO consumption due to H_2S oxidation	g O_2 m^{-3} d^{-1}
RNIT2DO	DO consumption due to nitrification	g O_2 m^{-3} d^{-1}
reLDOC2DO	DO consumption by mineralisation of LDOC	g O_2 m^{-3} d^{-1}
DEPC2DO	DO consumption by mineralisation during PC death	g O_2 m^{-3} d^{-1}
ODSC	Sediment DO consumption	g O_2 m^{-3} d^{-1}

ODPC: Net O_2 production/consumption by phytoplankton, g O_2 $m^{-3}d^{-1}$

$$ODPC = (PRPC1 + PRPC2 + PRPC3) * vo \quad (3.142)$$

REAR: Reaeration, surface layer only, g O_2 $m^{-3}d^{-1}$

$$REAR = IF\ depth<5\ THEN\ 0\ ELSE\ (3.93*\frac{\sqrt{hcur}}{depth^{1.5}} + \frac{2.07+0.215*wsp^{1.7}}{100*24})*(csair-DO)/dz \quad (3.143)$$

REAR1: Reaeration, shallow water all layers, g O_2 $m^{-3}d^{-1}$

$$REAR1 = IF\ depth<5\ THEN\ (3.93*\frac{\sqrt{hcur}}{MAX(0.1,depth)^{1.5}} + \frac{2.07+0.215*wsp^{1.7}}{100*24})*(csair-DO)*dz/depth\ ELSE\ 0 \quad (3.144)$$

ODDC: DO consumption by mineralisation of DC, g O_2 $m^{-3}d^{-1}$

$$ODDC = REDC * vo \quad (3.145)$$

ODZC: Zooplankton respiration, g O_2 $m^{-3}d^{-1}$

$$ODZC = REZC * vo \quad (3.146)$$

Where:

$$REZC = (GRPC1 + GRPC2 + GRPC3) * refo \quad (3.147)$$

SOXI2DO: DO consumption due to H_2S oxidation, g O_2 $m^{-3}d^{-1}$

$$SOXI2DO = SOXI * vsh \quad (3.148)$$

RNIT2DO: DO consumption due to nitrification, g O_2 $m^{-3}d^{-1}$

$$RNIT2DO = RNIT * vnh \quad (3.149)$$

reLDOC2DO: DO consumption by mineralisation of LDOC, g O_2 $m^{-3}d^{-1}$

$$reLDOC2do = reLDOC * vo \quad (3.150)$$

DEPC2DO: DO consumption by mineralisation during PC death, g O_2 $m^{-3}d^{-1}$

$$dDEPC2DO = (DEPC1 + DEPC2 + DEPC3) * vm * vo \quad (3.151)$$

ODSC: Sediment DO consumption, g O_2 $m^{-3}d^{-1}$

From the sediment-water intreface oxygen (DO) can penetrat into the sediment pore water by diffusion or actively being transportet into the sediment by ventilation pumping and sediment mixing by the benthic fauna. Further microbenthic algae through photosynthetis can produce DO in the sediment-waterinterface. DO is consumed in the sediment by bacterial respiration and chemical oxidation of reduced substances (Fe^{++}, H_2S) resulting in the O_2 concentration becomes 0 (normally 0-2 cm) below the sediment surface. In the model this depth is defined as KDO2. Assuming the DO produced by the microbenthic algae is delivered to the water, the below differential equation can be set up assuming a steady state condition:

$$0 = -difo2 * \frac{d^2 O_2}{dy^2} + DOconsum \quad (3.152)$$

Where 0<y<(KDO2), which by integration becomes:

$$\frac{d\ O_2}{dy} = \frac{DOconsum}{difo2} * y + a \quad (3.153)$$

Where a is a constant, which by using the border condition (dO_{2}/dy=0 at y=*KDO2*)) can be defined as:

$$a = -\frac{DOconsum}{difo2} * KDO2 \Rightarrow$$

$$\frac{d\,O_2}{dy} = \frac{DOconsum}{difo2} * y - \frac{DOconsum}{difo2} * KDO2 \quad (3.154)$$

Which by yet an integration gives:

$$O_2 = \frac{DOconsum}{2 * difo2} * y^2 - \frac{DOconsum}{difo2} * KDO2 * y + b \quad (3.155)$$

Where b is a constant, which by using the border condition (O_2=0 at y=KDO2) can be defined as:

$$b = \frac{DOconsum}{2*difno3} * KDO2^{\,2} \Rightarrow$$

$$O_2 = \frac{DOconsum}{2*difo2} * y^2 - \frac{DOconsum}{difo2} * KDO2 * y + \frac{DOconsum}{difo2} * KDO2^{\,2} \quad (3.156)$$

At the sediment surface y=0 the O_2 = DO =>

$$KDO2 = \sqrt{2 * difo2 * \frac{DO}{DOconsum}} \Rightarrow$$

$$O_2 = \frac{DOconsum}{2 * difo2} * y^2 - \frac{DOconsum}{difo2} * \sqrt{2 * difo2 * \frac{DO}{DOconsum}} * y + * 2 * DO \quad (3.157)$$

The flux of DO from the water into the sediment can be described using Fick's 1. Law at depth y=0

$$DOflux = -difo2 * \frac{dO_2}{dy} \quad (3.158)$$

$\frac{dO_2}{dy}$ is found by differentiation of the above expression for O_2 in the sediment and determaine the flux of DO into the sediment at Y=0.

$$DOflux = -difo2 * \left(-\frac{DOconsum}{difo2} * \sqrt{2 * difo2 * \frac{DO}{DOconsum}}\right) \Rightarrow$$

$$DOflux = \sqrt{2 * DO * difo2 * DOconsum} \Rightarrow \quad (3.159)$$

The DO consumption in the model is the sum of bacterial respiration (*reKDO2*), nitrification (rsnit) and a flux of reduced substances from the under laying sediment (*fsh2s*) to the layer with O_2. All the mentioned DO consuming processes has the unit (g $m^{-2}d^{-1}$) and therefore has to be divided with the DO penetration (KDO2). A conversion factor for O_2:N of 4.57 g O_2 :g NH_4-N is used and a conversion factor for O_2:S of 2 g O_2 : H_2S-S is used.

The diffusion or rather transport of oxygen into the sediment is dependent of the activity of the benthic infauna. Their activity is linked to the DO concentration, at low DO (below 2 g m^{-3}) the activity will decrease caused by increased mortality. The constant *difO2* is therefore multiplied by an oxygen function (1+sqdo).

The final equation for (ODSC, g O_2 $m^{-3}d^{-1}$) in the template therefore becomes:

$$ODSC = IF\ KDO2>0.001\ THEN \sqrt{2 * difO2 * (1 + sqdo) * DO * \frac{fsh2s * 2 + rsnit * 4.57 + reKDO2}{KDO2}} * \frac{1}{dz} \quad ELSE\ 0 \tag{3.160}$$

Where:

Name	Comment	Unit	Type*)
PRPC1	Production flagellate carbon	g C m^{-3} d^{-1}	P
PRPC2	Production diatom carbon	g C m^{-3} d^{-1}	P
PRPC3	Production cyanobacteria carbon	g C m^{-3} d^{-1}	P
vo	O_2:C ratio for Production & respiration	g O_2 g C^{-1}	C
hcur	Horizontal current	m s^{-1}	F
wsp	Wind speed, 10 m above sea	m s^{-1}	F
CSAIR	O_2 saturation in water, relative to PSU & temp.	g O_2 m^{-3}	A
DO	Oxygen in water	g O_2 m^{-3}	S
depth	Depth of water column	m	F
dz	Height of actual water layer	m	F
REDC	Respiration detritus	g C m^{-3} d^{-1}	P
REZC	Respiration zooplankton	g C m^{-3} d^{-1}	P
GRPC1	Grazing of phytoplankton (Flagellate) carbon	g C m^{-3} d^{-1}	P
GRPC2	Grazing of phytoplankton (diatom) carbon	g C m^{-3} d^{-1}	P
GRPC3	Grazing of cyanobacteria carbon	g C m^{-3} d^{-1}	P
refo	Zooplankton, respiration	g C g C^{-1}	C
SOXI	H_2S oxidation to SO_4	g S m^{-2} d^{-1}	P
vsh	O_2:S ratio for oxidation of H_2S to SO_4	g O_2 g S^{-1}	C
RNIT	Nitrification	g N m^{-3} d^{-1}	P

Name	Comment	Unit	Type*)
vnh	O_2:N ratio nitrification	g O_2 g N^{-1}	C
reLDOC	Respiration LDOC	g C m^{-3} d^{-1}	P
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
vm	Fraction of DEPC1-3 respired at once	n.u.	C
difO2	Diffusion of O2 in sediment	m^2 s^{-1}	C
DOconsum	Sediment O_2 consumption, layer (0-KDO2)	g O_2 $m^{-3}d^{-1}$	
y	Depth below sediment surface	m	
sqdo	DO dependend auxiliary	n.u.	A
fsh2s	H_2S flux from under laying anoxic sediment layer	g S m^{-2} d^{-1}	P
rsnit	Nitrification in sediment in oxic sediment layer	g N m^{-2} d^{-1}	P
reKDO2	Respiration in oxic sediment layer	g O m^{-2} d^{-1}	P1
KDO2	Oxic layer in sediment	m	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.23 CDOC, Coloured refractory DOC, g C m^{-3}

$$\frac{dCDOC}{dt} = depc2CDOC - phoxCDOC \tag{3.161}$$

Where:

Process	Comment	Unit
depc2CDOC	Fraction of depc to CDOC	g C m^{-3} d^{-1}
phoxCDOC	UV Photo oxidation of CDOC to LDOC	g C m^{-3} d^{-1}

depc2CDOC: Fraction of depc to CDOC, g C m^{-3} d^{-1}

$$depc2CDOC = (DEPC1 + DEPC2 + DEPC3) * vp \tag{3.162}$$

phoxCDOC: UV photo oxidation of CDOC to LDOC, g C m^{-3} d^{-1}

$$phoxCDOC = CDOC * doc_{maxde} * rd * doc_{monod} \quad (3.163)$$

Where:

Name	Comment	Unit	Type*)
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
vp	Fraction of DEPC, DEPN & DEPP to CDOC, CDON & CDOP	n.u.	C
doc_{maxde}	Max relative photo oxidation rate	d^{-1}	C
rd	Relative daylength, f(latitude, day,month,year)	n.u.	A
doc_{monod}	UV radiation Monod relation for photo oxidation	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.24 CDON, Coloured refractory DON, g N m^{-3}

$$\frac{dCDON}{dt} = depc2CDON - phoxCDON \quad (3.164)$$

Where:

Process	Comment	Unit
depc2CDON	Fraction of depn to CDON	g N m^{-3} d^{-1}
phoxCDON	UV Photo oxidation of CDON to LDON	g N m^{-3} d^{-1}

Depc2CDON: Fraction of depn to CDON, g N m^{-3} d^{-1}

$$depc2CDON = (DEPN1 + DEPN2 + DEPN3) * vp \quad (3.165)$$

phoxCDON: UV photo oxidation of CDON to LDON, g N m^{-3} d^{-1}

$$phoxCDON = CDON * doc_{maxde} * rd * doc_{monod} \quad (3.166)$$

Where:

Name	Comment	Unit	Type*)
DEPN1	Death of flagellate N	g N m^{-3} d^{-1}	P
DEPN2	Death of diatom N	g N m^{-3} d^{-1}	P
DEPN3	Death of cyanobacteria N	g N m^{-3} d^{-1}	P
vp	Fraction of depc, depn, depp to CDOC, CDON, CDOP	n.u.	C
rd	Relative daylength, f(latitude, day,month,year)	n.u.	A
doc_{maxde}	Max relative photo oxidation rate	d^{-1}	C
doc_{monod}	UV radiation Monod relation for photo oxidation	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.25 CDOP, Coloured refractory DOP, g P m^{-3}

$$\frac{dCDOP}{dt} = depc2CDOP - phoxCDOP \tag{3.167}$$

Where:

Process	Comment	Unit
depc2CDOP	Fraction of depp to CDOP	g P m^{-3} d^{-1}
phoxCDOP	UV Photo oxidation of CDOP to LDOP	g P m^{-3} d^{-1}

depc2CDOP: Fraction of depp to CDOP, g P m^{-3} d^{-1}

$$depc2CDOP = (DEPP1 + DEPP2 + DEPP3) * vp \tag{3.168}$$

phoxCDOP: UV photo oxidation of CDOP to LDOP, g P m^{-3} d^{-1}

$$phoxCDOP = CDOP * doc_{maxde} * rd * doc_{monod} \tag{3.169}$$

Where:

Name	Comment	Unit	Type*)
DEPP1	Death of flagellate P	g P m^{-3} d^{-1}	P
DEPP2	Death of diatom P	g P m^{-3} d^{-1}	P
DEPP3	Death of cyanobacteria P	g P m^{-3} d^{-1}	P
vp	Fraction of depc, depn, depp to CDOC, CDON, CDOP	n.u.	C
rd	Relative daylength, f(latitude, day,month,year)	n.u.	A
doc_{maxde}	Max relative photo oxidation rate	d^{-1}	C
doc_{monod}	UV radiation Monod relation for photo oxidation	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.26 LDOC, Labile DOC, g C m^{-3}

$$\frac{dLDOC}{dt} = phoxCDOC + depc2LDOC - reLDOC - deLDOC - sreLDOC \quad (3.170)$$

Where:

Process	Comment	Unit
phoxCDOC	UV Photo oxidation of CDOC to LDOC	g C m^{-3} d^{-1}
depc2LDOC	Fraction of depc to LDOC	g C m^{-3} d^{-1}
reLDOC	Aerobic respiration of LDOC using O_2	g C m^{-3} d^{-1}
deLDOC	Anaerobic respiration of LDOC using NO_3	g C m^{-3} d^{-1}
sreLDOC	Anaerobic respiration of LDOC using SO_4	g C m^{-3} d^{-1}

phoxCDOC: UV photo oxidation of CDOC to LDOC, g C m^{-3} d^{-1}

See under CDOC, Section 3.3.23.

depc2CDPC: Fraction of depc to LDOC, g C m^{-3} d^{-1}

$$depc2CDOC = (DEPC1 + DEPC2 + DEPC3) * vn \quad (3.171)$$

reLDOC: Aerobic respiration of LDOC using O_2, g C m^{-3} d^{-1}

$$reLDOC = LDOC * kmLC * tere^{T-20} * \frac{DO^{ndo2}}{DO^{ndo2} + mdo2} \quad (3.172)$$

deLDOC: Anaerobic respiration of LDOC using NO_3, g C m^{-3} d^{-1}

$$deLDOC = \frac{LDOC}{DC + LDOC} * (DENW * vn3 + ANAMOX * 0.429) \quad (3.173)$$

sreLDOC: Anaerobic respiration of LDOC using SO_4, g C m^{-3} d^{-1}

$$sreLDOC = \frac{LDOC}{DC + LDOC} * SRED * vso \quad (3.174)$$

Where:

Name	Comment	Unit	Type*)
DEPC1	Death of flagellate C	g C m^{-3} d^{-1}	P
DEPC2	Death of diatom C	g C m^{-3} d^{-1}	P
DEPC3	Death of cyanobacteria C	g C m^{-3} d^{-1}	P
vn	Fraction of depc, depn, depp to LDOC, LDON, LDOP	n.u.	C
tere	Θ in Arrhenius function, DC mineralisation	n.u.	C
ndo2	DC & LDOC:Coefficient, DO mineralisation	n.u.	C
mdo2	DO half-saturation constant, DC & LDOC mineralisation	n.u	C
kmLC	Specific mineralisation rate of LDOC at 20 °C	d^{-1}	C
DC	Detritus C	g C m^{-3}	S
DENW	Denitrification in water	g N m^{-3} d^{-1}	P
vn3	C:N ratio denitrification	g C g N^{-1}	C
sred	Anoxic C mineralisation via SO_4→H_2S	g S m^{-3} d^{-1}	P
vso	C:S ratio, SO_4 respiration	g C g S^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.27 LDON, Labile DON, g N m^{-3}

$$\frac{dLDON}{dt} = phoxCDON + depc2LDON - reLDON - deLDON - sreLDON \quad (3.175)$$

Where:

Process	Comment	Unit
phoxCDON	UV Photo oxidation of CDON to LDON	g N m^{-3} d^{-1}
depc2LDON	Fraction of depn to LDON	g N m^{-3} d^{-1}
reLDON	Aerobic respiration of LDON using O_2	g N m^{-3} d^{-1}
deLDON	Anaerobic respiration of LDON using NO_3	g N m^{-3} d^{-1}
sreLDON	Anaerobic respiration of LDON using SO_4	g N m^{-3} d^{-1}

phoxCDON: UV photo oxidation of CDON to LDON, g N m^{-3} d^{-1}

See under CDON, Section 3.3.24.

depc2LDON: Fraction of depn to LDON, g N m^{-3} d^{-1}

$$depc2CDON = (DEPN1 + DEPN2 + DEPN3) * vn \quad (3.176)$$

reLDON: Aerobic respiration of LDON using O_2, g N m^{-3} d^{-1}

$$reLDON = \frac{LDON}{LDOC} * reLDOC \quad (3.177)$$

deLDON: Anaerobic respiration of LDON using NO_3, g N m^{-3} d^{-1}

$$deLDON = \frac{LDON}{LDOC} * deLDOC \quad (3.178)$$

sreLDON: Anaerobic respiration of LDON using SO_4, g N m^{-3} d^{-1}

$$sreLDON = \frac{LDON}{LDOC} * sreLDOC \quad (3.179)$$

Where:

Name	Comment	Unit	Type*)
DEPN1	Death of flagellate P	g N m^{-3} d^{-1}	P
DEPN2	Death of diatom N	g N m^{-3} d^{-1}	P
DEPN3	Death of cyanobacteria N	g N m^{-3} d^{-1}	P
vn	Fraction of depc, depn, depp to LDOC, LDON, LDOP	n.u.	C
reLDOC	Aerobic respiration of LDOC using O_2	g C m^{-3} d^{-1}	P
deLDOC	Anaerobic respiration of LDOC using NO_3	g C m^{-3} d^{-1}	P
sreLDOC	Anaerobic respiration of LDOC using SO_4	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.3.28 LDOP, Labile DOP, g P m^{-3}

$$\frac{dLDOP}{dt} = phoxCDOP + depp2LDOP - UPLDOPP3 - reLDOP - deLDOP - sreLDOP \quad (3.180)$$

Where:

Process	Comment	Unit
phoxCDOP	UV Photo oxidation of CDOP to LDOP	g P m^{-3} d^{-1}
depp2LDOP	Fraction of depp to LDOP	g P m^{-3} d^{-1}
UPLDOPP3	Cyanobacteria uptake of LDOP	g P m^{-3} d^{-1}
reLDOP	Aerobic respiration of LDOP using O_2	g P m^{-3} d^{-1}
deLDOP	Anaerobic respiration of LDOP using NO_3	g P m^{-3} d^{-1}
sreLDOP	Anaerobic respiration of LDOP using SO_4	g P m^{-3} d^{-1}

phoxCDOP: UV photo oxidation of CDOP to LDOP, g P m^{-3} d^{-1}

See under CDOP, Section 3.3.25.

depp2LDOP: Fraction of depp to LDOP, g P m^{-3} d^{-1}

$$depp2CDOP = depp * vn \quad (3.181)$$

UPLDOPP3: Cyanobacteria uptake of LDOP, g P m^{-3} d^{-1}

Please see under state variable PP3, Section 3.3.9.

reLDOP: Aerobic respiration of LDOP using O_2, g P m^{-3} d^{-1}

$$reLDOP = \frac{LDOP}{LDOC} * reLDOC \tag{3.182}$$

deLDOP: Anaerobic respiration of LDOP using NO_3, g P m^{-3} d^{-1}

$$deLDOP = \frac{LDOP}{LDOC} * deLDOC \tag{3.183}$$

sreLDOP: Anaerobic respiration of LDOP using SO_4, g P m^{-3} d^{-1}

$$sreLDOP = \frac{LDOP}{LDOC} * sreLDOC \tag{3.184}$$

Where:

Name	Comment	Unit	Type*)
DEPP1	Death of flagellate P	g N m^{-3} d^{-1}	P
DEPP2	Death of diatom P	g N m^{-3} d^{-1}	P
DEPP3	Death of cyanobacteria P	g N m^{-3} d^{-1}	P
Vn	Fraction of depc, depn, depp to LDOC, LDON, LDOP	n.u.	C
reLDOC	Aerobic respiration of LDOC using O_2	g C m^{-3} d^{-1}	P
deLDOC	Anaerobic respiration of LDOC using NO_3	g C m^{-3} d^{-1}	P
sreLDOC	Anaerobic respiration of LDOC using SO_4	g C m^{-3} d^{-1}	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4 Differential Equation Sediment State Variables

3.4.1 SSi, Sediment, bio-available Silicate, g Si m^{23}

$$\frac{dSSi}{dt} = SESi - RSSi \tag{3.185}$$

Where:

Process	Comment	Unit
SESi	Deposition of Diatom & Detritus Si	g Si $m^{-2}d^{-1}$
RSSi	Flux of Si from sediment	g Si $m^{-2}d^{-1}$

SESi: Deposition of Diatom & Detritus Si, g Si $m^{-2}d^{-1}$

$$SESi = (SEPSi2 + SEDSi) * dz \tag{3.186}$$

RSSi: Flux of Si from sediment, g Si $m^{-2}d^{-1}$

$$RSSi = krss * trss^{T-20} * \frac{SSi}{SSi + hss1} * MAX(1, MIN\left(2, \frac{0.005}{KDOX}\right)) \tag{3.187}$$

Where:

Name	Comment	Unit	Type*)
SEPSi2	Sedimentation of diatom Si	g Si $m^{-3}d^{-1}$	P
SEDSi	Sedimentation of detritus Si	g Si $m^{-3}d^{-1}$	P
dz	Height of actual water layer	M	F
krss	Max Si release rate from sediment at 20 °C	g Si $m^{-2}d^{-1}$	C
trss	Θ value in Arrhenius temperature function, Si	n.u.	C
T	Temperature	°C	F
hss1	Half saturation constant for SSi	g Si m^{-2}	C
KDOX	NO_3 penetration depth in sediment	M	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.2 KDOX, depth of NO3 penetration in sediment, m

KDOX is the NO_3 penetration into the sediment. NO_3 is denitrified in the anoxic part of the sediment and therefore normally only penetrate 0-10 cm into the sediment. Normally, DO only penetrates a few mm into the sediment and therefore KDO2 (the DO penetration) will be smaller than KDOX. In a simulation, a situation may occur where KDOX is smaller than KDO2, which at least in theory may happen in nature. In this case, the increase in KDOX is set to a fixed fraction of the difference between KDO2 and KDOX.

$$\frac{dKDOX}{dt} = dkdox \tag{3.188}$$

Where:

Process	Comment	Unit
Dkdox	change oxidised layer sediment, KDOX	m d^{-1}

Change oxidised layer sediment, KDOX:

$$dkdox = \text{IF KDOX<KDO2 THEN } (KDOX - KDO2) * kkdox \text{ ELSE dkdox\_no3} \tag{3.189}$$

Where:

Name	Comment	Unit	Type*)
KDO2	DO penetration into sediment	m	S
kkdox	NO_3 penetration rate constant into sediment, KDOX<KDO2	d^{-1}	C
dkdox_no3	NO_3 penetration rate sediment, analytical solution	m d^{-1}	P1

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.3 KDO2, DO penetration in sediment, m

$$\frac{dKDO2}{dt} = dkdo2 \tag{3.190}$$

Where:

Process	Comment	Unit
dkdo2	change in DO penetration in sediment	m d^{-1}

dkdo2: Change in DO penetration in sediment, m d^{-1}

$$\begin{aligned} &dkdo2 = \text{IF (kds-KDO2)<epsi} \\ &\text{THEN} \\ &MIN(kdo2i - KDO2) * kkdo2,0) \\ &\text{ELSE} \\ &\text{(kdo2i-KDO2)*kkdo2} \end{aligned} \tag{3.191}$$

Where:

Name	Comment	Unit	Type*)
KDO2	DO penetration into sediment	m	S
kds	Depth of modelled sediment layer	m	C
epsi	Constant small value also used for PC nutrient uptake	n.u.	C
kdo2i	New steady state condition for KDO2, function of DO and respiration, analytical solution	m	P1
kkdo2	Rate constant for DO penetration into sediment	C	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.4 SOC, Sediment organic C, g C m^{-2}

$$\frac{dSOC}{dt} = depoC - minSOC - rscim \quad (3.192)$$

Where:

Process	Comment	Unit
depoC	Deposition of C	g C $m^{-2}d^{-1}$
minSOC	Mineralisation of SOC	g C $m^{-2}d^{-1}$
Rscim	Burial of sediment organic C	g C $m^{-2}d^{-1}$

Deposition of C on sediment surface:

$$depoC = (\text{SEPC1-BUOYC1+SEP2+SEPC3-BUOYC3+SEDC})*\underline{dz} \quad (3.193)$$

Where:

Name	Comment	Unit	Type*)
SEPC1	Sedimentation of flagellate C	g C m^{-3} d^{-1}	P
SEPC2	Sedimentation of diatom C	g C m^{-3} d^{-1}	P
SEPC3	Sedimentation of cyanobacteria C	g C m^{-3} d^{-1}	P
BUOYC1	Flagellate upward movement	g C m^{-3} d^{-1}	P
BUOYC3	Cyanobacteria upward movement	g C m^{-3} d^{-1}	P
SEDC	Sedimentation of detritus C (DC) to sediment	g C m^{-3} d^{-1}	P
Dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

minSOC: Mineralisation of SOC, g C $m^{-2}d^{-1}$

$$minSOC = \text{krsc1*SOC*}tetn^{T-20} + \text{fscb*dz} \quad (3.194)$$

Where:

Name	Comment	Unit	Type*)
krsc1	Specific mineralisation rate of SOC 20 °C	d^{-1}	C
tetn	Θ in Arrhenius temperature equation, SON mineralisation	n.u.	C
temp	Temperature	°C	F
fscb	Mineralisation of newly settled organic C	g C $m^{-3}d^{-1}$	P1
Dz	Height of actual layer= layer above sediment	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

rscim: Burial of sediment organic C, g C $m^{-2}d^{-1}$

$$rscim = (depoC - fscb * dz) * \frac{rsnim}{rson} \quad (3.195)$$

Where:

Name	Comment	Unit	Type*)
depoC	Deposition of C	g C $m^{-2}d^{-1}$	P
Fscb	Mineralisation of newly settled organic C	g C $m^{-3}d^{-1}$	P1
Rsnim	Burial of organic sediment N (SON), see SON (Section 3.4.5)	g N $m^{-2}d^{-1}$	P
Rson	Burial of organic sediment N (SON), see SON (Section 3.4.5)	g N $m^{-2}d^{-1}$	P
Dz	Height of actual layer= layer above sediment	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.5 SON, Bio-available organic N in sediment, g N m^{-2}

$$\frac{dSON}{dt} = rson - rsonnh - rsnim \tag{3.196}$$

Where:

Process	Comment	Unit
Rson	Settling of organic N to SON	g N $m^{-2}d^{-1}$
Rsonnh	Mineralisation of SON to pore water NH_4	g N $m^{-2}d^{-1}$
Rsnim	Burial of organic sediment N (SON)	g N $m^{-2}d^{-1}$

rson: Settling of organic N to SON

$$rson = (SEPN1 - \boldsymbol{BUOYN1} + SEPN2 + SEPN3 - \boldsymbol{BUOYN3} + SEDN - fsnb) * dz \tag{3.197}$$

Where:

Name	Comment	Unit	Type*)
SEPN1	Sedimentation of flagellate N	g N m^{-3} d^{-1}	P
SEPN2	Sedimentation of diatom N	g N m^{-3} d^{-1}	P
SEPN3	Sedimentation of cyanobacteria N	g N m^{-3} d^{-1}	P
BUOYN1	Flagellate upward movement N	g N m^{-3} d^{-1}	P
BUOYN3	Cyanobacteria upward movement N	g N m^{-3} d^{-1}	P
SEDN	Sedimentation of detritus N, (DN), see DN	g N m^{-3} d^{-1}	P
Fsnb	Mineralisation of newly settled organic N on sed. surface	g N m^{-3} d^{-1}	P1
Dz	Height of actual layer= layer above sediment	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

rsonnh: Mineralisation of SON to pore water NH_4

$$rsonh = krsn1 * SON * tetn^{T-20} \quad (3.198)$$

Where:

Name	Comment	Unit	Type*)
krsn1	Specific mineralisation rate of SON 20 °C	d^{-1}	C
Tetn	Θ in Arrhenius temperature equation, SON mineralisation	n.u.	C
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

rsnim: Burial of organic sediment N (SON), g N $m^{-2}d^{-1}$

The mineralisation of SOC and SON is assumed to a function of the sediment SON:SOC ratio. At low SON:SOC ratios close to *knim* the mineralisation is assumed to small or close to 0. The fraction of organic N settled to the sediment (*rson*) to buried or immobilised is set to be *knim* multiplied with settled organic C to sediment. If N:C ration of the settled N is below *knim* all settled N (rson) is buried.

$$\begin{aligned} &rsnim = IF\ knim * (depoC - fscb * dz) < rson \\ &THEN \\ &knim * (depoC - fscb * dz) \\ &\text{ELSE} \\ &\text{Rson} \end{aligned} \quad (3.199)$$

Where:

Name	Comment	Unit	Type*)
knim	Sediment: N:C ratio of immobile N	g N g C^{-1}	C
depoC	Deposition of C, see SOC	g C $m^{-2}d^{-1}$	P
fscb	Mineralisation of newly settled organic C	g C $m^{-3}d^{-1}$	P1
rson	Settling of organic N to SON	g N $m^{-2}d^{-1}$	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.6 SOP, Bio-available organic P in sediment, g P m^{-2}

$$\frac{dSOP}{dt} = rsop - ropsip - rspim \quad (3.200)$$

Where:

Process	Comment	Unit
rsop	Settling of organic P to SOP	g P $m^{-2}d^{-1}$
ropsip	Mineralisation of SOP to pore water PO_4	g P $m^{-2}d^{-1}$
rspim	Burial – immobilisation of organic sediment P (SOP)	g P $m^{-2}d^{-1}$

rsop: Settling of organic P to SOP, g P $m^{-2}d^{-1}$

$$rsop = (SEPP1 - \boldsymbol{BUOYP1} + SEPP2 + SEPP3 - \boldsymbol{BUOYP3} + SEDP - fspb) * dz \quad (3.201)$$

Where:

Name	Comment	Unit	Type*)
SEPP1	Sedimentation of flagellate P	g P m^{-3} d^{-1}	P
SEPP2	Sedimentation of diatom P	g P m^{-3} d^{-1}	P
SEPP3	Sedimentation of cyanobacteria P	g P m^{-3} d^{-1}	P
BUOYP1	Flagellate upward movement P	g P m^{-3} d^{-1}	P
BUOYP3	Cyanobacteria upward movement P	g P m^{-3} d^{-1}	P
Fspb	Mineralisation of newly settled organic P on sed. Surface	g P m^{-3} d^{-1}	P1
Dz	Height of actual layer= layer abowe sediment	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

ropsip: Mineralisation of SOP to pore water PO_4, g P $m^{-2}d^{-1}$

$$ropsip = krsp1 * SOP * tetp^{T-20} \quad (3.202)$$

Where:

Name	Comment	Unit	Type*)
krsp1	Specific mineralisation rate of SOP 20 °C	d^{-1}	C
tetp	Θ in Arrhenius temperature equation, SOP mineralisation	n.u.	C
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

rspim: Burial and immobilisation of organic sediment P (SOP), g P $m^{-2}d^{-1}$

P is able to be incorporated into hydroxyapatite (chalk) or adsorbed to reduced Fe (in fresh waters) or simply it is incorporated into inert organic C. The processes are not well known and therefore a fixed fraction of the settled organic P is immobilised. In sediments (typical marine) where the pool of H2S (reduced substances) exceeds a fixed value of 0.01 g S m-2 immobilisation to Fe++ is reduced to 1/10.

The user may change the process if new information is available, or information on sediment type prescribes another formulation.

$$rspim = IF\ H2S > 0.01\ THEN\ \frac{kpim}{10} * rsop\ ELSE\ kpim * rsop \quad (3.203)$$

Where:

Name	Comment	Unit	Type*)
knim	Sediment: P:C ratio of immobile P	g P g C^{-1}	C
rsop	Settling of organic P to SOP	g N $m^{-2}d^{-1}$	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.7 FESP, PO4 adsorbed to oxidised ion in sediment, g P m^{-2}

$$\frac{dFESP}{dt} = rfesip \tag{3.204}$$

Where:

Process	Comment	Unit
rfesip	Flux between pore water PO_4 and iron-absorped P	g P $m^{-2}d^{-1}$

rfesip: Flux between pore water PO_4 and iron-absorped P, g P $m^{-2}d^{-1}$

The exchange of PO_4-P between oxidised ion (Fe^{+++}) is calculated as a rate constant (*krap*) multiplied with the difference between a new steady state sorption of PO_4 to Fe+++ ($FESP\_f(KDOX)_\infty$) and the last calculated pool of sorbed PO_4-P ($FESP_t$).

An approximation of $FESP\_f(KDOX)_\infty$ is estimated using a Monod kinetic for PO_4 in the pore water combined with information of sediment ion conten, dry matter sediment, density and finaly multiplied with the oxidised layer (KDOX), which is a state variable in the model.

$$rfesip = krap * (FESP\_f(KDOX)_\infty - FESP_t) \quad =>$$

$$rfesip = krap * (kfe * kfepo * \frac{SIPm3}{SIPm3 + khfe} * vf * dm * KDOX * 10^6 - FESP) \tag{3.205}$$

Where:

Name	Comment	Unit	Type*)
krap	Rate constant for iron absorption – desorption of PO_4	d^{-1}	C
kfe	Oxidable ion content in sediment	g Fe g dw^{-1}	C
Kfepo	Maximum Fe-P sorption capacity	g P g Fe^{-1}	C
SIPm3	Pore water PO_4 concentration	g P m^{-3}	A
khfe	Half saturation constant, adsorption-desorption	g P m^{-3}	C
vf	Sediment density	g WW cm^{-3}	C
dm	Dry weight sediment	g DM g WW^{-1}	C
KDOX	Depth of No3 penetration ~oxidised layer with Fe^{+++}	m	S
FESP	Ion(FE^{+++}) bound PO4 in sediment	g P m^{-2}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.8 SNH, Sediment pore water NH4, g N m^{-2}

$$\frac{dSNH}{dt} = rsonnh - rsnit - feunh4 \quad (3.206)$$

Where:

Process	Comment	Unit
rsonnh	Mineralisation of SON to pore water NH_4	g N m^{-2}d^{-1}
rsnit	Nitrification of NH_4 in sediment	g N m^{-2}d^{-1}
feunh4	NH_4 Flux between sediment pore water and water	g N m^{-2}d^{-1}

rsonnh: mineralisation of SON to pore water NH_4, g N m^{-2}d^{-1}

Please see under the state variable SON, Section 3.4.5.

rsnit: Nitrification of NH_4 in sediment, g N m^{-2}d^{-1}

The nitrification of NH4 in sediment pore water (*SNHm3*) is described as the product between a specific nitrification rate (knit), SNHm3, a Monod relation of *SNHm3* a Monod relation for DO (*sqdo*), the DO penetration in the sediment (*KDO2*) and a temperature relation.

$$rsnit = \text{IF DO}>0 \text{ THEN } knit * SNHm3 * \frac{SNHm3}{SNHm3 + ksnh0} * sqdo * KDO2 * tetn^{T-20} \text{ ELSE } 0 \quad (3.207)$$

Where:

Name	Comment	Unit	Type*)
Knit	Specific nitrification rate at 20 C in sediment	d^{-1}	C
SNHm3	NH_4 concentration in pore water	g N m^{-3}	A
ksnh0	NH_4 half saturation concentration for nitrification	g N m^{-3}	C
Sqdo	DO Mond function	n.u.	A
KDO2	DO penetration in sediment	m	S
Tetn	Θ in Arrhenius temperature equation, SON mineralisation	n.u.	C
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

feunh4: NH_4 Flux between sediment pore water and water, g N $m^{-2}d^{-1}$

The flux between pore water NH_4 (*SNHm3*) and NH_4 in the water (*NH4*) is described as a product of a vertical diffusion constant (*difnh*) and concentration difference divided with the the NO_3 penetration depth in the sediment (*KDOX*).

$$feunh4 = difnh * \frac{SNHm3 - NH4}{MIN(kds, KDOX)} \quad (3.208)$$

Where:

Name	Comment	Unit	Type*)
difnh	Vertical diffusion for ammonia	m^2d^{-1}	C
SNHm3	NH_4 concentration in pore water	g N m^{-3}	A
NH4	NH_4 concentration in water	g N m^{-3}	C
kds	Depth of modelled sediment layer	m	C
KDOX	NO_3 penetration in sediment~oxidised layer	m	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.9 SNO3, NO3 in sediment pore water, layer (0 - kdo2), g N m^{-2}

$$\frac{dSNO3}{dt} = rsnit - rdenit - feuno3 \quad (3.209)$$

Where:

Process	Comment	Unit
rsnit	Nitrification of pore water NH_4 in sediment	g N $m^{-2}d^{-1}$
Rdenit	Denitrification of NO_3 in sediment	g N $m^{-2}d^{-1}$
feuno3	NO_3 Flux between sediment pore water and water	g N $m^{-2}d^{-1}$

rsnit: Nitrification of pore water NH_4 in sediment, g N $m^{-2}d^{-1}$

Please see state variable SNH, Section 3.4.8.

rdenit: Denitrification of NO_3 in sediment, g N $m^{-2}d^{-1}$

rdenit is expressed as flux of NO_3 into the anoxic zone of the sediment where only diffusion and denitrification are the driving processes. An analytical solution is used assuming steady state conditions.

From the surface layer of the sediment with DO (*KDO2*), NO_3 in the pore water with concentration S*NO3m3* will penetrate deeper into the anoxic sediment layer while being denitrified to N_2. At a sudden depth below the surface (*KDOX*) NO_3 concentration will be 0. Assuming a constant denitrification and under steady state condition the NO_3 concentration (*NO3x)* in the pore water at depth x below the surface layer with DO can be described with:

$$0 = -difno3 * \frac{d^2 NO3x}{dx^2} + dnm3 \text{ Where } 0<x<(KDOX-KDO2) \quad (3.210)$$

Which by integration becomes:

$$\frac{d\ NO3x}{dx} = \frac{dnm3}{difno3} * x + a \quad (3.211)$$

Where a is a constant, which by using the border condition (*dNO3x/dx*=0 at x=(*KDOX-KDO2)*) can be defined as:

$$a = -\frac{dnm3}{difno3} * (KDOX - KDO2) \Rightarrow$$
$$\frac{d\ NO3x}{dx} = \frac{dnm3}{difno3} * (x - (KDOX - KDO2)) \quad (3.212)$$

Which by yet an integration gives:

$$NO3x = \frac{dnm3}{2 * difno3} * x^2 * - \frac{dnm3}{difno3} * (KDOX - KDO2) * x + b \quad (3.213)$$

Where b is a constant, which by using the border condition (*SNO3m3*=0 at x=(*KDOX-KDO2)*) can be defined as:

$$b = \frac{dnm3}{2*difno3} * (KDOX - KDO2)^2 \Rightarrow$$
$$NO3x = \frac{dnm3}{2*difno3} * x^2 - \frac{dnm3}{difno3} * (KDOX - KDO2) * x + \frac{dnm3}{2*difno3} * (KDOX - KDO2)^2 \quad (3.214)$$

At depth x=0 in the anoxic zone (which is at depth KDO2 below sediment surface) *NO3x=SNO3m3*. =>

$$(KDOX - KDO2) = \sqrt{2 * difno3 * \frac{SNO3m3}{dnm3}} \Rightarrow$$
$$NO3x = \frac{dnm3}{2 * difno3} * x^2 - \frac{dnm3}{difno3} * \sqrt{2 * difno3 * \frac{SNO3m3}{dnm3}} * x + 2 * SNO3m3 \quad (3.215)$$

Assuming the flux of NO_3 into the anoxic sediment solely being created by denitrification the NO_3-flux=denitrification pr. m^2 d^{-1} = rdenit.

Using Fick's 1. law for a flux at depth x=0.

$$rdenit = -difno3 * \frac{dNO3x}{dx} \quad (3.216)$$

$\frac{dNO3x}{dx}$ is found by differentiation of the above expression for *NO3x* and determine the flux for x=0. The final equation used in the template:

$$rdenit = \sqrt{2 * difno3 * dnm3 * SNO3m3} \quad (3.217)$$

Where:

Name	Comment	Unit	Type*)
difno3	Vertical diffusion for NO_3 in sediment	m^2d^{-1}	C
dnm3	denitrification in sediment, corrected for temperature	g N $m^{-3}d^{-1}$	A
SNO3m3	NO_3 in pore water surface sediment, layer (0-kdo2)	g N m^{-3}	A
KDO2	DO penetration into the sediment	m	S
KDOX	NO_3 penetration into the sediment	m	S
NO3x	NO_3 concentration in pore water at depth x	g N m^{-3}	
X	Depth below zone with DO	m	

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

feuno3: NO_3 Flux between sediment pore water and water, g N $m^{-2}d^{-1}$

The flux between pore water NO_3 (*SNO3m3*) and NO_3 in the water (*NO3*) is described as a product of a vertical diffusion constant (*difno3*) and concentration difference divided with the the DO penetration depth in the sediment (*KDO2*).

$$feuno3 = difno3 * \frac{SNO3m3 - NO3}{KDO2} \quad (3.218)$$

Where:

Name	Comment	Unit	Type*)
difno3	Vertical diffusion for NO_3 in sediment	m^2d^{-1}	C
NO3	NO_3 concentration in water	g N m^{-3}	S
SNO3m3	NO_3 in pore water surface sediment, layer (0-kdo2)	g N m^{-3}	A
KDO2	DO penetration into the sediment	m	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.10 SIP, PO4 in sediment pore water, g P m^{-2}

$$\frac{dSIP}{dt} = -rfesip + ropsip - fsip \tag{3.219}$$

Where:

Process	Comment	Unit
rfesip	Flux between pore water PO_4 and iron-adsorbed P	g P $m^{-2}d^{-1}$
ropsip	Mineralisation of SOP to pore water PO_4	g P $m^{-2}d^{-1}$
fsip	Flux between PO_4 in pore water and water above sediment	g P $m^{-2}d^{-1}$

rfesip: Flux between pore water PO_4 and iron-absorped P, g P $m^{-2}d^{-1}$

Please see under the stat variable FESP, sediment ion adsorbed PO_4, Section 3.4.7.

ropsip: Mineralisation of SOP to pore water PO_4, g P $m^{-2}d^{-1}$

Please see under the stat variable SOP, bio-available organic P in sediment. Section 3.4.6.

fsip: Flux between PO_4 in pore water and water above sediment, g P $m^{-2}d^{-1}$

The flux between pore water PO_4 (*SIPm3*) and PO_4 in the water (IP) is described as a product of a vertical diffusion constant (*kfip*) and concentration difference divided with the NO_3 penetration depth in the sediment (*KDOX*).

$$fsip = kfip * \frac{SIPm3 - IP}{KDOX} \tag{3.220}$$

Where:

Name	Comment	Unit	Type*)
kfip	Vertical diffusion for PO_3 in sediment	m^2d^{-1}	C
IP	PO_4 concentration in water	g N m^{-3}	S
SIPm3	PO_4 in pore water of the sediment	g N m^{-3}	A
KDOX	NO_3 penetration into the sediment	m	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.11 SH2S, Reduced substances in sediment, g S m^{-2}

$$\frac{dH2S}{dt} = RSH2S - fsh2s - fwsh2s \quad (3.221)$$

Where:

Process	Comment	Unit
RSH2S	Sediment H2S production in anaroxic layer: mineralisation of SOC – denitrification	g S $m^{-2}d^{-1}$
fsh2s	flux of SH2S from reduced sediment (below KDOX) to oxidised sediment.	g S $m^{-2}d^{-1}$
fwsh2	flux of reduced H2S equivalents from sediment to water	g S $m^{-2}d^{-1}$

RSH2S: Sediment H2S production in anaroxic layer: mineralisation of SOC minus denitrification

The production of H2S (reduced substances in sediment expressed as H_2S-S) is calculated as the mineralisation of SOC (minSOC) minus the a fraction of the minSOC being oxidised by DO in layer KDO2 minis a fraction of minSOC being oxidised by NO_3 by denitrification in the anoxic zone penetrated by NO_3 (KDOX-KDO2). A C:N ratio of 1.07 is used to convert denitrified NO_3-N to C, and a C:S ratio of 1.33 is used to convert mineralised C to S.

$$RSH2S = \left(minSOC - \frac{erKDO2}{vo} - rdenit * 1.07\right) * 1.33 \quad (3.222)$$

Where:

Name	Comment	Unit	Type*)
minSOC	mineralisation SOC	g C $m^{-2}d^{-1}$	P
reKDO2	Sediment mineralisation of SOC by DO, in layer KDO2	g O_2 $m^{-2}d^{-1}$	P1
Vo	O_2: C ratio used in production & consumption processes	g O_2 g C^{-1}	C
Rdenit	Denitrification in anoxic sediment layer	g N $m^{-2}d^{-1}$	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fsh2s: flux of SH2S from reduced sediment (below KDOX) to oxidised sediment, g S $m^{-2}d^{-1}$

The flux of reduced substances expressed as H_2S-S from sediment below the oxidised zone of the sediment (below KDOX) is expressed as a diffusion constant multiplied by a H_2S concentration difference between the H_2S concentration (calculated from SH2S) and the H2S concentration in the water above the sediment divided by the distance from the reduced zone in the sediment to the depth of DO penetration (KDO2).

$$\begin{array}{l} fsh2s = IF\ KDO2 > 0.001 \\ THEN \\ \quad difh2s * \dfrac{\dfrac{SH2S}{(1-dm) * vf * \left(kds - MAX\left(KDO2, (KDOX - KDO2)\right)\right)} - H2S}{KDOX - KDO2} \\ ELSE\ 0 \end{array} \tag{3.223}$$

Where:

Name	Comment	Unit	Type*)
difh2s	Vertical diffusion of SH2S in sediment	m^2d^{-1}	C
SH2S	Reduced substances in sediment as H_2S	g S m^{-2}	S
vf	Sediment density	g WW cm^{-3}	C
dm	Dry weight sediment	g DM g WW^{-1}	C
kds	Depth of modelled sediment layer	m	C
KDO2	DO penetration into the sediment	m	S
KDOX	NO_3 penetration into the sediment	m	S
H2S	Hydrogen sulphide in water above sediment (H_2S)	g S m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fwsh2s: flux of reduced H2S equivalents from sediment to water, g S m^{-2} d^{-1}
In case the DO penetration in the sediment (KDO2) is below 1 mm the flux of H_2S go directly from the reduced zone of the sediment into the water above the sediment.

$$fwsh2s = IF\ KDO2 \leq 0.001$$
$$THEN$$
$$difh2s * \frac{\frac{SH2S}{(1-dm)*vf*(kds-KDO2)} - H2S}{KDOX} \quad (3.224)$$
$$ELSE\ 0$$

Where:

Name	Comment	Unit	Type*)
difh2s	Vertical diffusion of SH2S in sediment	m^2d^{-1}	C
SH2S	Reduced substances in sediment as H_2S	g S m^{-2}	S
Vf	Sediment density	g WW cm^{-3}	C
Dm	Dry weight sediment	g DM g WW^{-1}	C
Kds	Depth of modelled sediment layer	m	C
KDO2	DO penetration into the sediment	m	S
KDOX	NO_3 penetration into the sediment	m	S
H2S	Hydrogen sulphide in water above sediment (H_2S)	g S m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.12 SPIM, Immobilised sediment P, g P m^{-2}

$$\frac{dSPIM}{dt} = rspim \quad (3.225)$$

Where:

Process	Comment	Unit
Rspim	Immobilisation of sediment P	g P $m^{-2}d^{-1}$

rspim: Immobilisation of sediment P, g P $m^{-2}d^{-1}$

The immobilisation of P in the sediment is set to be a constant fraction of the organic P settling to the sediment surface. In water bodies with permanently or semi permanent anoxia having a H_2S concentration above 0.01 g S m^{-3} the immobilisation is set to be 10% of

$$rspim = IF\ H2S > 0.01\ THEN$$

$$\frac{kpim}{10} * rsop \qquad (3.226)$$

$$ELSE\ \ kpim * rsop$$

Where:

Name	Comment	Unit	Type*)
H2S	H_2S in the water above the sediment	g S m^{-3}	S
kpim	Fraction of settled P to immobilisation	n.u.	C
rsop	Supply of organic P to sediment	g P $m^{-2}d^{-1}$	P

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.4.13 SNIM, Immobilised sediment N by denitrification & burial, g N m^{-2}

$$\frac{dSNIM}{dt} = rsnim + rdenit \qquad (3.227)$$

Where:

Process	Comment	Unit
rspim	Immobilisation of sediment N by burial	g N $m^{-2}d^{-1}$
rdenit	Denitrification of NO_3 in sediment	g N $m^{-2}d^{-1}$

rsnim: Immobilisation of sediment N by burial, g N $m^{-2}d^{-1}$

Please see under state variable sediment organic N (SON), Section 3.4.5.

rdenit: Denitrification of NO_3 in sediment, g N $m^{-2}d^{-1}$

Please see under state variable sediment NO3 (SN03), Section3.4.9.

3.4.14 SNIM, Immobilised sediment N by denitrification & burial, g N m^{-2}

$$\frac{dSCIM}{dt} = minSOC + rscim \tag{3.228}$$

Where:

Process	Comment	Unit
minSOC	Mineralisation of SOC	g C $m^{-2}d^{-1}$
rscim	Burial of sediment organic C	g C $m^{-2}d^{-1}$

minSOC: Mineralisation of SOC, g C $m^{-2}d^{-1}$

Please see under state variable sediment organic C (SOC), Section 3.4.4.

rscim: Burial of sediment organic C, g C $m^{-2}d^{-1}$

Please see under state variable sediment organic C (SOC), Section 3.4.4.

3.5 Help Processes

The help processes are divided into processes not included into differential equations (P1) and auxiliary processes (A). The distinction between is unimportant and relay on P1 processes in ECO Lab being able to be defined exclusively for bottom layer, surface layer and all layers in a 3D model. This distinction is not possible for auxiliary processes.

3.5.1 The P1 processes listed in alphabetic order

dkdox_no3: Change in NO3 penetration rate sediment, analytical solution, m d^{-1}

NO_3 in the pore water of the sediment is caused by penetration of NO_3 form water above the sediment and by nitrification of NH_4 in the uppermost layer (KDO2) with DO in the pore water. The NO_3 concentration in this layer (0 to KDO2) has in the model the average concentration S*NO3m3.* From this layer NO_3 penetrates deeper into the anoxic sediment layer while being denitrified to N_2. Provided there is no outflow of NO_3 enriched ground water the NO_3 concentration at a sudden depth below the surface (*KDOX*) will be 0. Assuming a constant denitrification and under steady state condition the NO_3 concentration (*NO3x)* in the pore water at depth x below the surface layer with DO can be described with:

$$0 = -difno3 * \frac{d^2 NO3x}{dx^2} + dnm3 \text{ Where } 0<x<(KDOX_{\infty}\text{-}KDO2) \quad (3.229)$$

Which by integration becomes:

$$\frac{d\ NO3x}{dx} = \frac{dnm3}{difno3} * x + a \quad (3.230)$$

Where a is a constant, which by using the border condition (*dNO3x/dx*=0 at x=(*KDOX-KDO2)*) can be defined as:

$$a = -\frac{dnm3}{difno3} * (KDOX_{\infty} - KDO2) \Rightarrow$$

$$\frac{d\ NO3x}{dx} = \frac{dnm3}{difno3} * (x - (KDOX_{\infty} - KDO2)) \quad (3.231)$$

Which by yet an integration gives:

$$NO3x = \frac{dnm3}{2*difno3} * x^2 - \frac{dnm3}{difno3} * (KDOX_{\infty} - KDO2) * x + b \quad (3.232)$$

Where b is a constant, which by using the border condition (*SNO3m3*=0 at x=(*KDOX*$_{\infty}$*-KDO2)*) can be defined as:

$$b = \frac{dnm3}{2*difno3} * (KDOX_{\infty} - KDO2)^2 \Rightarrow$$

$$NO3x = \frac{dnm3}{2*difno3} * x^2 - \frac{dnm3}{difno3} * (KDOX_{\infty} - KDO2) * x + \frac{dnm3}{2*difno3} * (KDOX_{\infty} - KDO2)^2 \quad (3.233)$$

At depth x=0 in the anoxic zone (which is at depth KDO2 below sediment surface) *NO3x=SNO3m3*. =>

$$(KDOX_{\infty} - KDO2) = \sqrt{2 * difno3 * \frac{SNO3m3}{dnm3}} \Rightarrow$$

$$KDOX_{\infty} = \sqrt{2 * difno3 * \frac{SNO3m3}{dnm3}} + KDO2 \quad (3.234)$$

$KDOX_{\infty}$ in the above equation is the NO_3 peneteration in the sediment under steady state condition. Assuming $KDO2_t$ ~$KDO2_{t+1}$ the change in the change in in KDOX (kdox_no3) from time step t to time step t+1 can the be defined as:

$$dkdox_{no3} = (KDOX_{\infty} - KDOX_t) * kkdox$$

$$dkdox_{no3} = \left(\sqrt{2 * difno3 * \frac{SNO3m3}{dnm3}} + KDO2_t - KDOX_t\right) * kkdox \quad (3.235)$$

Where:

Name	Comment	Unit	Type*)
difno3	Vertical diffusion for NO_3 in sediment	m^2d^{-1}	C
dnm3	denitrification in sediment, corrected for temperature	g N $m^{-3}d^{-1}$	A
SNO3m3	NO_3 in pore water surface sediment, layer (0-kdo2)	g N m^{-3}	A
KDO2	DO penetration into the sediment	m	S
$KDO2_t$	DO penetration into the sediment , time step t	m	
KDOX	NO_3 penetration into the sediment, same as $KDOX_t$	m	S
kkdox	Rate constant NO_3 penetration into sediment	d^{-1}	C
$KDOX_t$	NO_3 penetration into the sediment, time step t	m	
$KDOX_{\infty}$	NO_3 penetration into the sediment, steady state	m	
NO3x	NO_3 concentration in pore water at depth x	g N m^{-3}	
x	Depth below zone with DO	m	

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fscb: Mineralisation of newly settled organic C, g C $m^{-3}d^{-1}$

A fraction of newly settled particulate organic C (plankton and detritus) on the sediment surface is assumed to be mineralised at once. The fraction mineralised is dependent on the N:C ratio.

$$fscb = \frac{fsnb}{SEPN1 - BUOYN1 + SEPN2 + SEPN3 - BUOYN3 + SEDN} * \frac{depoC}{dz} \quad (3.236)$$

Where:

Name	Comment	Unit	Type*)
fsnb	Mineralisation of newly settled organic N	g N $m^{-3}d^{-1}$	P1
depoC	Deposition of particulate organic C	g C $m^{-2}d^{-1}$	P
SEPN1	Sedimentation of flagellate N	g N m^{-3} d^{-1}	P
SEPN2	Sedimentation of diatom N	g N m^{-3} d^{-1}	P
SEPN3	Sedimentation of cyanobacteria N	g N m^{-3} d^{-1}	P
BUOYN1	Flagellate upward movement N	g N m^{-3} d^{-1}	P
BUOYN3	Cyanobacteria upward movement N	g N m^{-3} d^{-1}	P
SEDN	Deposition of detritus N	g N $m^{-3}d^{-1}$	P
dz	Height of actual layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fsnb: Mineralisation of newly settled organic N, g N $m^{-3}d^{-1}$

A fraction of newly settled particulate organic N (plankton, detritus and dead eelgrass) on the sediment surface is assumed to be mineralised at once. The fraction mineralised is dependent on the N:C ratio.

$$fsnb = krsn0 * \left(SEPN1 - BUOYN1 + SEPN2 + SEPN3 - BUOYN3 + SEDN - \frac{depoC * knim}{dz}\right) * tetn^{temp-20} \quad (3.237)$$

Where:

Name	Comment	Unit	Type*)
krsn0	Fraction of deposited N mineralised	d^{-1}	C
depoC	Deposition of particulate organic C	g C $m^{-2}d^{-1}$	P
SEPN1	Sedimentation of flagellate N	g N m^{-3} d^{-1}	P

Name	Comment	Unit	Type*)
SEPN2	Sedimentation of diatom N	g N m^{-3} d^{-1}	P
SEPN3	Sedimentation of cyanobacteria N	g N m^{-3} d^{-1}	P
BUOYN1	Flagellate upward movement N	g N m^{-3} d^{-1}	P
BUOYN3	Cyanobacteria upward movement N	g N m^{-3} d^{-1}	P
SEDN	Deposition of detritus N	g N $m^{-3}d^{-1}$	P
dz	Height of actual layer	m	F
knim	Sediment N:C ratio of immobile N	g N g C^{-1}	C
tetn	Θ value in Arrhenius temperature function	n.u.	C
temp	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fspb: Mineralisation of newly settled organic P, g P $m^{-3}d^{-1}$

A fraction of newly settled particulate organic P (plankton and detritus) on the sediment surface is assumed to be mineralised at once. The fraction mineralised is not set to be dependent on the N:C ratio, because mineralised P as PO_4 can be adsorbed to resuspended fine sediment containing Fe^{+++}. The user should therefore consider this problem and set the constant *krsp0* accordingly, from model set up to model set up.

$$fspb = krsp0 * (SEPP1 - SUOYP1 + SEPP2 + SEPP3 - BUOYP3 + SEDP) * tetp^{temp-20} \quad (3.238)$$

Where:

Name	Comment	Unit	Type*)
krsp0	Fraction of deposited N mineralised	d^{-1}	C
SEPP1	Sedimentation of flagellate P	g P m^{-3} d^{-1}	P
SEPP2	Sedimentation of diatom P	g P m^{-3} d^{-1}	P
SEPP3	Sedimentation of cyanobacteria P	g P m^{-3} d^{-1}	P
BUOYP1	Flagellate upward movement P	g P m^{-3} d^{-1}	P
BUOYP3	Cyanobacteria upward movement P	g P m^{-3} d^{-1}	P
SEDP	Deposition of detritus P	g P $m^{-3}d^{-1}$	P
tetp	Θ value in Arrhenius temperature function	n.u.	C
temp	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

kdo2i: new steady state condition for KDO2, function of DO & respiration, analytical solution

From the sediment-water intreface oxygen (DO) can penetrat into the sediment pore water by diffusion or actively being transportet into the sediment by ventilation pumping and sediment mixing by the benthic fauna. Further microbenthic algae through photosynthetis can produce DO in the sediment-water interface. DO is consumed in the sediment by bacterial respiration and chemical oxidation of reduced substances (Fe^{++}, H_2S) resulting in the O_2 concentration becomes 0 (normally 0-2 cm) below the sediment surface. In the model this depth is defined as KDO2. Assuming the DO produced by the microbenthic algae is delivered to the water, the below differential equation can be set up assuming a steady state condition:

$$0 = -difo2 * \frac{d^2 O_2}{dy^2} + DOconsum \text{ Where } 0<y<(KDO2_\infty) \tag{3.239}$$

Which by integration becomes:

$$\frac{d\ O_2}{dy} = \frac{DOconsum}{difo2} * y + a \tag{3.240}$$

Where a is a constant, which by using the border condition ($dO_{2/dy}$=0 at y=$KDO2_\infty$) can be defined as:

$$a = -\frac{DOconsum}{difo2} * KDO2_\infty \Rightarrow$$

$$\frac{d\ O_2}{dy} = \frac{DOconsum}{difo2} * y - \frac{DOconsum}{difo2} * KDO2_\infty \tag{3.241}$$

Which by yet an integration gives:

$$O_2 = \frac{DOconsum}{2 * difo2} * y^2 - \frac{DOconsum}{difo2} * KDO2_\infty * y + b \tag{3.242}$$

Where b is a constant, which by using the border condition (O_2=0 at y=$KDO2_\infty$) can be defined as:

$$b = \frac{DOconsum}{2*difno3} * KDO2_\infty{}^2 \Rightarrow$$

$$O_2 = \frac{DOconsum}{2*difo2} * y^2 - \frac{DOconsum}{difo2} * KDO2_\infty * y + \frac{DOconsum}{difo2} * KDO2_\infty{}^2 \tag{3.243}$$

At the sediment surface y=0 the O_2 = DO =>

$$KDO2_\infty = \sqrt{2 * difo2 * \frac{DO}{DOconsum}} \Rightarrow \tag{3.244}$$

$KDO2_\infty$ is identical to *ko2i* in the model, however the DO consumption in the model is the sum of bacterial respiration (*reKDO2*), nitrification (rsnit) and a flux of reduced substances from the under laying sediment (*fsh2s*) to the layer with O_2. All the mentioned DO consuming processes has the unit (g $m^{-2}d^{-1}$) and therefore has to be divided with the DO penetration from the previous time step t ($KDO2_t$). A conversion factor for O_2:N of 4.57 g O_2:g NH_4-N is used and a conversion factor for O_2:S of 2 g O_2 : H_2S-S is used.

The diffusion or rather transport of oxygen into the sediment is dependent of the activity of the benthic infauna. Their activity is linked to the DO concentration, at low DO (below 2 g m^{-3}) the activity will decrease caused by increased mortality. The constant *difO2* is therefore multiplied by an oxygen function (1+sqdo).

$$kdo2i = \sqrt{2 * DO * \frac{difo2 * (1 + sqdo) * KDO2_t}{(rsnit * 4.57 + reKDO2 + fsh2s * 2)}} \quad (3.245)$$

Where:

Name	Comment	Unit	Type*)
difo2	Vertical diffusion for O_2 in sediment, low fauna activity	m^2d^{-1}	C
DOconsum	Sediment O_2 consumption, layer (0-KDO2)	g O_2 $m^{-3}d^{-1}$	
y	Depth below sediment surface	m	
$KDO2_\infty$	DO penetration into the sediment, steady state=***kdo2i***	m	
$KDO2_t$	DO penetration into the sediment time step t=***KDO2***	m	
KDO2	DO penetration into the sediment	m	S
sqdo	DO dependend auxiliary	n.u.	A
rsnit	Nitrification in sediment layer (0-KDO2)	g N $m^{-2}d^{-1}$	P
reKDO2	DO consumption by bacteria layer (0-KDO2)	g O_2 $m^{-2}d^{-1}$	P1
fsh2s	Flux of SH2S from reduced sediment to layer (0-KDO2)	g S $m^{-2}d^{-1}$	P
DO	O_2 in water above sediment	g O_2 m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

reKDO2: Sediment mineralisation of SOC by DO, in layer KDO2, g O_2 m^{-2} d^{-1}

$$reKDO2 = \frac{KDO2}{kds} * minSOC * vo * sqdo \quad (3.246)$$

Where:

Name	Comment	Unit	Type*)
KDO2	DO penetration depth in sediment	m	S
kds	Depth of modelled sediment layer	m	C
minSOC	Mineralisation of organic in sediment	g C m^{-2} d^{-1}	P
vo	O_2 : C ration production, respiration, mineralisation	g O_2 g C $^{-1}$	C
sqdo	Oxygen function	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

3.5.2 Auxiliary (A) processes listed in alphabetic order

buoy1: N & P & light upward movement function, flagellate, n.u.

The upward movements of phytoflagellates are a function of the light regime and nutrient condition of the algae. If the internal N and P pools (N/C and P/C ratios in the algae) are small the function powNP1 will have a small but positive value resulting in an in sedbouNP1 being negative and the buoy1 becoming 0. At low powNP1 there will be no upward movements. At high powNP1values (high N/C and P/C ratio in the algae) sedbouNP1 become positive and the algae will move upward provided the light doze is below a value of kiz3.

buoy1=IF i≤kiz3
THEN MAX (0,sedbouNP1) (3.247)
ELSE 0

Where:

$$sedbuoNP1 = k2NP * (\frac{powNP1}{powNP1 + k3NP^{k1NP}} - 0.5) \quad (3.248)$$

And:

$$powNP1 = MIN(myp1, myn1)^{k1NP} \quad (3.249)$$

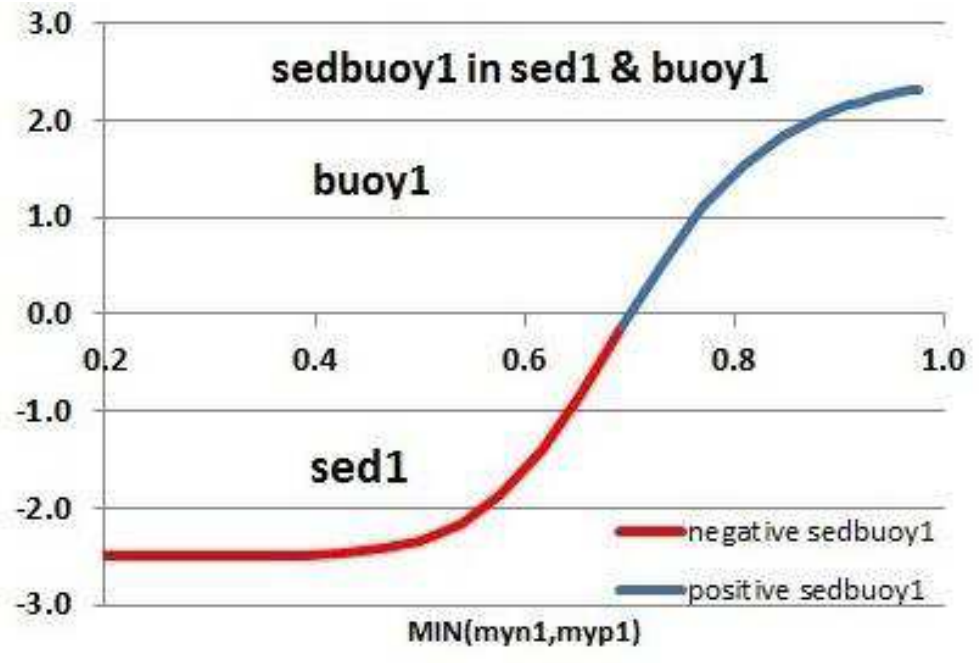

Figure 3.3 Figure Flagellates upward movement is dependent of positive values of sedboy1, which is dependent on a good N and P condition myn1 and myp1

Where:

Name	Comment	Unit	Type*)
kiz3	Light limit, buoyancy for PC1 & PC 3	mol photon $m^{-2}d^{-1}$	C
i	Photosynthetic Active Light (PAR) at top of layer	mol photon $m^{-2}d^{-1}$	A
k1NP	Exponent, sedimentation & buoyancy, PC1&PC3	n.u.	C
k2NP	Factor, sedimentation & buoyancy, PC1 & PC3	n.u.	C
k3NP	Shift from sedimentation to buoyancy, PC1 & PC3	n.u.	C
powNP1	Power function limiting nutrient, Flagellate (PC1)	n.u.	A
myn1	Nitrogen function flagellates	n.u.	A
myp1	Phosphorous function flagellates	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

buoy3: N & P & light upward movement function, cyanobacteria, n.u.

The upward movement of cyanobacteria is a function of the light regime and nutrient condition of the bacteria. If the internal N and P pools (N/C and P/C ratios in the bacteria) are small the function powNP3 will have a small but positive value resulting in an in sedbouNP3 being negative and the buoy1 becoming 0. At low powNP3 there will be no upward movements. At high powNP3 values (high N/C and P/C ratio in the bacteria) sedbouNP3 become positive and the algae will move upward provided the light doze is below a value of *kiz3*.

$$buoy3=IF\ i\leq kiz3\ THEN\ MAX(0,sedbouNP3)\ ELSE\ 0 \tag{3.250}$$

Where:

$$sedbuoNP3 = k2NP * (\frac{powNP3}{powNP3 + k3NP^{k1NP}} - 0.5) \tag{3.251}$$

And:

$$powNP3 = MIN(myp3, myn3)^{k1NP} \tag{3.252}$$

Where:

Name	Comment	Unit	Type*)
kiz3	Light limit, buoyancy for PC1 & PC 3	mol photon $m^{-2}d^{-1}$	C
i	Photosynthetic Active Light (PAR) at top of layer	mol photon $m^{-2}d^{-1}$	A
k1NP	Exponent, sedimentation& buoyancy, PC1&PC3	n.u.	C
k2NP	Factor, sedimentation & buoyancy, PC1 & PC3	n.u.	C
k3NP	Shift from sedimentation to buoyancy, PC1 & PC3	n.u.	C
powNP3	Power function limiting nutrient, cyanobacteria	n.u.	A
myn3	Nitrogen function cyanobacteria	n.u.	A
myp3	Phosphorous function cyanobacteria	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

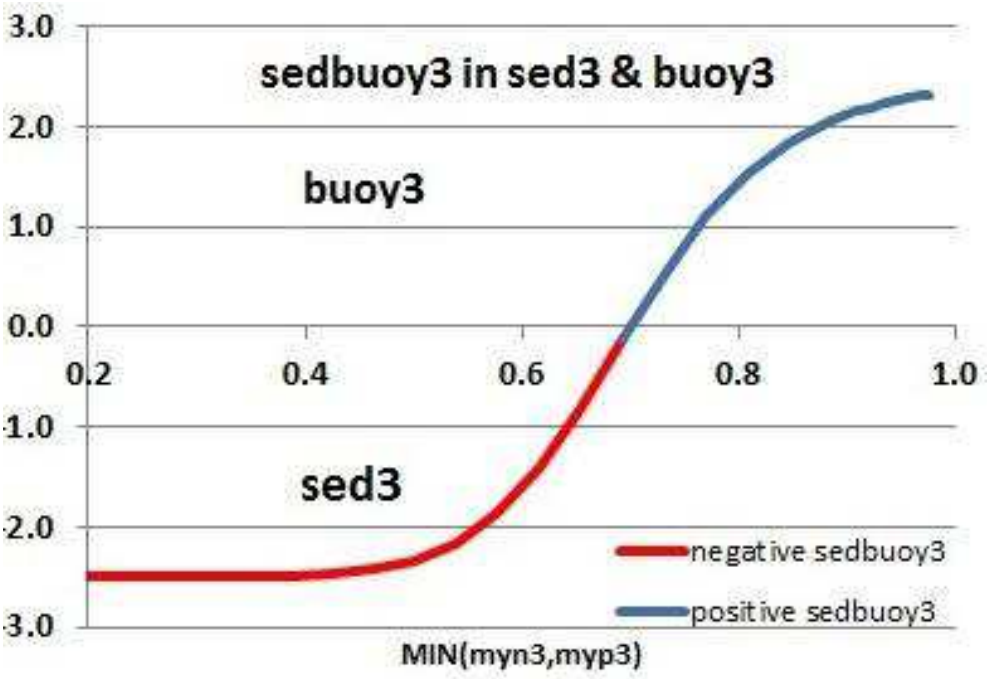

Figure 3.4 Cyanobaterial upward movement is dependent of positive values of sedboy3, which is dependent on a good N and P condition myn3 and myp3.

CSAIR: O_2 saturation in water, relative to PSU & temp., g O_2 m^{-3}

A built in function in ECO Lab calculates the O_2 saturation relative to salinity and temperature. In this template the O2 saturation defined by (Weiss 1970) is used:

CSAIR= OXYGENSATURATION_WEISS(S,T) (3.253)

Or:

$$CSAIR=\frac{e^{a}}{0.69997} \quad (3.254)$$

Where:

$$a=-173.4292+249.6339+\frac{100}{T+273.15}+143.2483*\log\left(\frac{T+273.15}{100}\right)-21.8493*\left(\frac{T+273.15}{100}\right)+S*\left(-0.033096+0.014259*\frac{T+273.15}{100}-0.0017*\left(\frac{T+273.15}{100}\right)^{2}\right) \quad (3.255)$$

In other templates the below equation is used.

CSAIR= OXYGENSATURATION(S,T) (3.256)

Or:

CSAIR= 14. 65 – 0 0841 · S + T*(0. 00256 · S – 0. 41022 + T*(0.007991-0.0000374*S -0. 000077774*T)) (3.257)

Where:

Name	Comment	Unit	Type*)
S	Salinity	PSU	F
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

dndc: N:C ration, detritus, g N g C^{-1}

$$dndc = \frac{DN}{DC} \tag{3.258}$$

Where:

Name	Comment	Unit	Type*)
DN	Detritus N	g N m^{-3}	S
DC	Detritus C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

dnm3: denitrification in sediment, corrected for temperature

$$dnm3 = demax * tetn^{T-20} \tag{3.259}$$

Where:

Name	Comment	Unit	Type*)
Demax	Max. denitrification rate in sediment at 20 °C	g N $m^{-2}d^{-1}$	C
Tetn	Θ value in Arrhenius temperature function	n.u	C
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

doc_{monod}: UV radiation Monod relation for photo oxidation, n.u.

$$DOC_{monod} = \frac{i - doc_{ie}}{i - doc_{ie} + doc_{ik}} \quad (3.260)$$

Where:

Name	Comment	Unit	Type*)
I	Solar radiation (PAR) in actual water column layer	µmol photon m^{-2} s^{-1}	A
doc_{ie}	min PAR light, CDOC photo oxidation	µmol photon m^{-2} s^{-1}	C
doc_{ik}	PAR half saturation photo oxidation of CODC	µmol photon m^{-2} s^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

dpdc: P:C ration, detritus, g P g C^{-1}

$$dndc = \frac{DP}{DC} \quad (3.261)$$

Where:

Name	Comment	Unit	Type*)
DP	Detritus P	g P m^{-3}	S
DC	Detritus C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

dsidc: Si:C ration, detritus, g Si g C^{-1}

$$dSidc = \frac{DSi}{DC} \quad (3.262)$$

Where:

Name	Comment	Unit	Type*)
DSi	Detritus Si	g Si m^{-3}	S
DC	Detritus C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

DT_{day}: AD time step (and not HD time step!) in days, d step^{-1}

$$DT_{day} = \frac{DT}{86400} \tag{3.263}$$

Where:

Name	Comment	Unit	Type*)
DT	Time step in sec.	Sec. step^{-1}	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

eta: Vertical light attenuation, m^{-1}

It is possible to calculate the vertical light attenuation based on light extinction constants or use the expression formulated by (Effer 1988; Kirk 2000) splitting the light attenuation into a light absorption and a scattering of light.

The surface area of the particles are important for the optical properties, as small particle have a larger surface area, they also have a higher vertical light extinction constant or a higher light scattering constant. In general the optical properties of particulate matter are proportional to the surface area of the particles in the water. In the equation for **eta1** and scattering **scatw** 3 size classes of inorganic matter (ss1-ss3) are defined in g m^{-3}. The mass is not an ideal measure for inorganic matter in relation to the optical properties; therefore the mass of ss1-ss3 is related to a particle size with a diameter of 10 µm, by multiplication of a factor (10/diass$_x$). Small particles below 10 µm thereby will be assigned a higher light extinction constant, or absorption and scattering constants, whereas larger particles will be assigned smaller constants.

The shape of the particles may be anything from a ball to spherical cone; therefore the correction factor (10/diass$_x$) should only be regarded as guidelines to be used if no measured data exists.

In the present ECO Lab template resuspension is not included therefore the light extinction not included dynamically in the model often is put into the background light extinction (bla) and the light extinction form suspended matter is the light extinction from marine earth works. The user should in this case be aware that the background extinction varies in time and space especially in coastal waters.

$$\text{eta} = IF\ Keta > 0\ THEN\ eta2\ ELSE\ eta1 \tag{3.264}$$

Where:

$$\text{eta1} = pla * CH + dla * DC + cla * CDOC + sla * 10 * \left(\frac{ss1}{diass1} + \frac{ss2}{diass2} + \frac{ss3}{diass3}\right) + bla \tag{3.265}$$

$$\text{eta2} = \sqrt{absw^2 + 0.256 * absw * scatw}$$

And:

$$\text{absw} = pla_a * CH + dla_a * DC + cla_a * CDOC + sla_a * 10 * \left(\frac{ss1}{diass1} + \frac{ss2}{diass2} + \frac{ss3}{diass3}\right) + bla_a \quad (3.266)$$

$$\text{scatw} = bkch * CH^{ekch} + bkss * \left(\frac{10*SS1}{diass1} + \frac{10*ss2}{diass2} + \frac{10*ss3}{diass3}\right)^{ekss}$$

The scatter of light (scatw) is defined as a power function of phytoplankton chlorophyll, (Morel A. 1980, Prieur L. & S. Sathyendranath 1981). The authours found a value range for bkch of 0.12-0.4 $m^2 mg^{-1}$ & ekch 0.63. The scatter by phytoplankton is dependent on cell size. The cell size tends to be smaller at low chlorophyll concentrations, where the plankton typically is nutrient limited (Yentsch C.S., D. A. Phinney 1989).

Lund-Hansen L.C. 2004 found chlorophyll in average to be responsible for 41% of the scattering in the nearby Århus Bay using a fixed specific chlorophyll scattering of 0.239 $m^2 mg^{-1}$ measured in New Zeland coastal waters (Pfannkuche F. 2002).

Please note that the mentioned scatter constants should be converted from m^2mg^{-1} to m^2g^{-1} before being used in this model.

Where:

Name	Comment	Unit	Type*)
Keta	Constant for choice of eta estimate	n.u.	C
eta1	Function vertical light attenuation, extinction constants	m^{-1}	A
eta2	Function vertical light attenuation, absorption & scattering	m^{-1}	A
pla	Chlorophyll light extinction constant	$m^2 g^{-1}$	C
CH	Chlorophyll concentration	$g m^{-3}$	S
dla	Detritus light extinction constant	$m^2 g^{-1}$	C
DC	Detritus C	$g m^{-3}$	S
cla	CDOC light extinction constant	$m^2 g^{-1}$	C
CDOC	Coloured refractory DOC	$g m^{-3}$	S
sla	Inorganic matter light extinction constant (Θ=10 µm)	$m^2 g^{-1}$	C
ss1	Inorganic matter, s e class 1	$g m^{-3}$	F
ss2	Inorganic matter, size class 2	$g m^{-3}$	F
ss3	Inorganic matter, size class 3	$g m^{-3}$	F
diass1	Diameter of inorganic matter, size class 1	µm	C
diass2	Diameter of inorganic matter, size class 2	µm	C

Name	Comment	Unit	Type*)
diass2	Diameter of inorganic matter, size class 2	µm	C
bla	Background light extinction	m^{-1}	C
absw	Light absorption in layer	m^{-1}	A
scatw	Light scattering in layer	m^{-1}	A
pla_a	Chlorophyll light absorption constant	$m^2 g^{-1}$	C
dla_a	Detritus light absorption constant	$m^2 g^{-1}$	C
cla_a	CDOC light absorption constant	$m^2 g^{-1}$	C
sla_a	Inorganic matter light absorption constant (Θ=10 µm)	$m^2 g^{-1}$	C
bla_a	Background light absorption	m^{-1}	C
bkch	Chlorophyll scattering constant	$m^2 g^{-1}$	C
ekch	Chlorophyll scattering exponent	n.u.	C
bkss	Inorganic matter scattering constant	$m^2 g^{-1}$	C
ekss	Inorganic matter scattering exponent	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fiz: Light factor for flagellates and cyanobacteria (PC1 & PC3) sedimentation, n.u.

$$fiz = fiz1 * fiz2 \tag{3.267}$$

Where:

$$fiz1 = IF\ i > kiz1\ THEN\ 3\ ELSE\ 1$$

$$fiz2 = IF\ i > kiz2\ THEN\ 1\ ELSE\ 0 \tag{3.268}$$

Where:

Name	Comment	Unit	Type*)
fiz1	1. Help factor for PC1 & PC3 sedimentation	n.u.	A
fiz2	2. Help factor for PC1 & PC3 sedimentation	n.u.	A
i	Light at top of actual water layer	mol photon $m^{-2}d^{-1}$	A
kiz1	Light limit for 3 X sedimentation rate of PC1 & PC3	mol photon $m^{-2}d^{-1}$	C
kiz2	Light limit for 1 X sedimentation rate of PC1 & PC3	mol photon $m^{-2}d^{-1}$	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fiz1: 1. Help factor for PC1 & PC3 sedimentation, n.u.

See under auxiliary fiz, Equation (3.18) and Equation (3.29).

fiz2: 2. Help factor for PC1 & PC3 sedimentation, n.u.

See under auxiliary fiz, Equation (3.18) and Equation (3.29).

fn3a: Denitrification, DO dependency in water column, n.u.

$$fn3a = \frac{ksb}{ksb + DO} \tag{3.269}$$

Where:

Name	Comment	Unit	Type*)
ksb	Denitrification Half saturation conc. DO	g $O_2 m^{-3}$	C
DO	Oxygen concentration	g $O_2 m^{-3}$	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fp3sal: Function for cyanobacteria dependency (death & growth) of salinity, n.u.

$$fp3sa = IF\ S < kp3opti\ THEN\ 1\ ELSE\ e^{-kp3sal1*(S-kp3sal2)} \tag{3.270}$$

Where:

Name	Comment	Unit	Type*)
kp3opti	Highest salinity for optimum cyanobacteria growth	PSU	C
kp3sal1	Cyanobacteria growth salinity dependency coefficient	PSU^{-1}	C
kp3sal2	Cyanobacteria growth salinity dependency constant	PSU	C
S	Salinity	PSU	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

fsa: Salinity function for reduction of SO_4 to H_2S, n.u.

$$fsa = IF\ S > ksa\ THEN\ 1\ ELSE\ 0 \tag{3.271}$$

Where:

Name	Comment	Unit	Type*)
ksa	Minimum salinity for SO_4 reduction	PSU	C
S	Salinity	PSU	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

i: Solar radiation (PAR) in actual water column layer (j), mol photon $m^{-2}d^{-1}$

If the surface water temperature >0.2 °C the water is assumed ice free and i_0 will be the light (PAR) reaching the surface of the water.

If the temperature is below 0.2 °C ice is assume on the water and only 10% of i_0 is assumed to penetrate the ice cover.

In a more general form the light (PAR) distribution in the different water layer can be expressed as:

$$i = i_o * e^{\sum_j^0 -eta_{0-j} * dz_{0-j}} \tag{3.272}$$

ECO Lab has an builtin function (LAMBERT_BEER_1) calculate the light (PAR) at the top of each water layer.

The average light (PAR) in a water layer can be expressed as:

$$i = \frac{1 - e^{-eta*dz}}{eta * dz} * LAMBERT\_BEER\_1(i_0, dz, eta) \tag{3.273}$$

Where:

Name	Comment	Unit	Type*)
i_o	Solar (PAR) radiation at water surface	mol photon $m^{-2}d^{-1}$	F
eta_{0-j}	Light attenuation (Kd) in layers 0 to j	m^{-1}	
dz_{0-j}	Height of layer 0 to j	m	
eta	Light attenuation (Kd) in actual layer	m^{-1}	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

ik1: Temperature corrected Light saturation for flagellates, mol photon $m^{-2}d^{-1}$

$$ik1 = alfa1 * teti^{T-20} \quad (3.274)$$

Where:

Name	Comment	Unit	Type*)
alfa1	Light saturation at 20 °C for flagellates	mol photon $m^{-2}d^{-1}$	C
teti	Θ value Arrhenius expression	n.u	C
T	temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

ik2: Temperature corrected Light saturation for diatoms, mol photon $m^{-2}d^{-1}$

$$ik2 = alfa2 * teti^{T-20} \quad (3.275)$$

Where:

Name	Comment	Unit	Type*)
Alfa2	Light saturation at 20 °C for diatoms	mol photon $m^{-2}d^{-1}$	C
teti	Θ value Arrhenius expression	n.u	C
T	temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

ik3: Temperature corrected Light saturation for cyanobacteris, mol photon $m^{-2}d^{-1}$

$$ik3 = alfa3 * teti^{T-20} \quad (3.276)$$

Where:

Name	Comment	Unit	Type*)
Alfa3	Light saturation at 20 °C for cyanobacteria	mol photon $m^{-2}d^{-1}$	C
teti	Θ value Arrhenius expression	n.u	C
T	temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

ksd: Sedimentation rate detritus, d^{-1}

The sedimentation of a particle is not allowed to pass through several water layers in one time step (DT_{day} time step in d). The sedimentation in one times step is therefore restricted to a maximum of dz. This is valid for ECO Lab version 2011 and earlier.

This restriction may led to an underestimation of sedimentation in 3-D set ups with a fine vertical resolution using small dz. However by not imposing the below restriction in sedimentation will potentially generate mass balance errors.

$$ksd = IF\ dz \leq sevd * DT_{day}\ THEN\ \frac{dz}{DT_{day}}\ ELSE\ sevd \tag{3.277}$$

Where:

Name	Comment	Unit	Type*)
dz	Height of actual water layer	m	F
DT_{day}	AD time step	d $step^{-1}$	C
sevd	Sedimentation rate	m d^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mgpc: Temperature, O_2 & food corrected max. grazing rate by zooplankton, d^{-1}

$$mgpc = kgrb * tetz^{T-20} * \frac{sqdo}{1 + e^{kgrm - kgrs*(kedib1*PC1 + kedib2*PC2 + kedib3*PC3)}} \tag{3.278}$$

Where:

Name	Comment	Unit	Type*)
kgrb	Max. specific grazing rate, zooplankton	d^{-1}	C
tetz	Θ in Arrhenius temp. relation of zooplankton grazing	n.u.	C
T	Temperature	°C	F
sqdo	DO function	n.u.	A
kgrm	Zooplankton 0. order dependency of grazing on plankton	n.u.	C
kgrs	Zooplankton 1. order dependency of grazing on plankton	n.u.	C
kedib1	Edible fraction of Flagellate	n.u.	C
kedib2	Edible fraction of Flagellate	n.u.	C

Name	Comment	Unit	Type*)
kedib3	Edible fraction of Flagellate	n.u.	C
PC1	Flagellate C	g C m^{-3}	S
PC2	Diatom C	g C m^{-3}	S
PC3	Cyanobacteria C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mnl1: Nutrient dependent death factor, flagellate, n.u.

The death factor is 1 with flagellate having high internal N:C and P:C ratios, but up to 5 in a nutrient stressed condition (low N:C and P:C ratios).

$$mnl1 = MIN(\frac{\left(\frac{1}{myn1} + \frac{1}{myp1}\right)}{2}, 5) \quad (3.279)$$

Where:

Name	Comment	Unit	Type*)
myn1	Nitrogen function flagellate	n.u	A
myp1	Phosphorous function flagellate	n.u	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mnl2: Nutrient dependent death factor, diatoms, n.u.

The death factor is 1 with diatoms having high internal N:C, P:C and Si:C ratios, but up to 5 in a nutrient stressed condition (low N:C, P:C or Si:C ratios).

$$mnl2 = MIN(\frac{\left(\frac{1}{myn2} + \frac{1}{myp2} + \frac{1}{mys2}\right)}{3}, 5) \quad (3.280)$$

Where:

Name	Comment	Unit	Type*)
myn2	Nitrogen function diatoms	n.u	A
myp2	Phosphorous function diatoms	n.u	A
mys2	Si function, diatoms	n.u	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mnl3: Nutrient dependent death factor, cyanobacteria, n.u.

The death factor is 1 with cyanobacteria having high internal N:C and P:C ratios, but up to 5 in a nutrient stressed condition (low N:C and P:C ratios).

$$mnl3 = MIN(\frac{\left(\frac{1}{myn3} + \frac{1}{myp3}\right)}{2}, 5) \quad (3.281)$$

Where:

Name	Comment	Unit	Type*)
myn3	Nitrogen function cyanobacteria	n.u	A
myp3	Phosphorous function cyanobacteria	n.u	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mntp1: N, P & temperature corrected max. net growth rate, flagellates d^{-1}

$$mntp1 = myte1 * \frac{2}{\left(\frac{1}{myn1} + \frac{1}{myp1}\right)} \quad (3.282)$$

Where:

Name	Comment	Unit	Type*)
myte1	Specific growth ,temperature regulated, flagellates	n.u.	A
myn1	Nitrogen function flagellates	n.u.	A
myp1	Phosphorous function flagellates	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mntp2: N, P & temperature corrected max. net growth rate, diatoms d^{-1}

$$mntp2 = myte2 * \frac{3}{\left(\frac{1}{myn2} + \frac{1}{myp2} + \frac{1}{mys2}\right)} \quad (3.283)$$

Where:

Name	Comment	Unit	Type*)
myte2	Specific growth ,temperature regulated, diatoms	n.u.	A
myn2	Nitrogen function diatoms	n.u.	A
myp2	Phosphorous function diatoms	n.u.	A
mys2	Silicate function diatoms	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mntp3: N, P & temperature corrected max. net growth rate, cyanobacteria d^{-1}

$$mntp3 = myte3 * \frac{2}{\left(\frac{1}{myn3} + \frac{1}{myp3}\right)} \quad (3.284)$$

Where:

Name	Comment	Unit	Type*)
myte3	Specific growth ,temperature regulated, cyanobacteria	n.u.	A
myn3	Nitrogen function cyanobacteria	n.u.	A
myp3	Phosphorous function cyanobacteria	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mspc1: Sedimentation rate flagellate phytoplankton, d^{-1}

The sedimentation of a particle is not allowed to pass through several water layers in one time step (DT_{day} time step in d). The sedimentation in one times step is therefore restricted to a maximum of dz. This is valid for ECO Lab version 2011 and earlier.

$$mspc1 = IF\ dz \leq seve1 * DT_{day}\ THEN\ \frac{dz}{DT_{day}}\ ELSE\ seve1 \quad (3.285)$$

This restriction may lead to an underestimation of sedimentation in 3D set-ups with a fine vertical resolution using small dz. However, by not imposing the above restriction in sedimentation will potentially generate mass balance errors.

Where:

Name	Comment	Unit	Type*)
seve1	Sedimentation rate flagellate	m d^{-1}	C
DT_{day}	**AD** time step (and not HD time step!) in days	d	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mspc2: Sedimentation rate diatom phytoplankton, d^{-1}

The sedimentation of a particle is not allowed to pass through several water layers in one time step (DT_{day} time step in d). The sedimentation in one times step is therefore restricted to a maximum of dz. This is valid for ECO Lab version 2011 and earlier.

$$mspc2 = IF\ dz \leq seve2 * DT_{day}\ THEN\ \frac{dz}{DT_{day}}\ ELSE\ seve2 \tag{3.286}$$

This restriction may lead to an underestimation of sedimentation in 3D set-ups with a fine vertical resolution using small dz. However, by not imposing the above restriction in sedimentation will potentially generate mass balance errors.

Where:

Name	Comment	Unit	Type*)
seve2	Sedimentation rate diatoms	m d^{-1}	C
DT_{day}	**AD** time step (and not HD time step!) in days	d	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mspc3: Sedimentation rate cyanobacteria, d^{-1}

The sedimentation of a particle is not allowed to pass through several water layers in one time step (DT_{day} time step in d). The sedimentation in one times step is therefore restricted to a maximum of dz. This is valid for ECO Lab version 2011 and earlier.

$$mspc3 = IF\ dz \leq seve3 * DT_{day}\ THEN\ \frac{dz}{DT_{day}}\ ELSE\ seve3 \tag{3.287}$$

This restriction may lead to an underestimation of sedimentation in 3D set-ups with a fine vertical resolution using small dz. However, by not imposing the above restriction in sedimentation will potentially generate mass balance errors.

Where:

Name	Comment	Unit	Type*)
seve3	Sedimentation rate cyanobacteria	m d^{-1}	C
DT_{day}	**AD** time step (and not HD time step!) in days	d	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myfi1: Light function Flagellate, n.u.

Equation (3.288) is an analytical solution of the integrated light available for production of flagellates in the water column.

Where:

$$myfi1 = (zk1 + \frac{i}{ik1 * eta} * (e^{-eta*zk1} - e^{-eta*dz}))/dz \quad (3.288)$$

Where:

Name	Comment	Unit	Type*)
zk1	Light availability flagellate production	m	A
ik1	Light saturation flagellate temperature corrected	mol photon $m^{-2}d^{-1}$	A
eta	Vertical light attenuation	m^{-1}	A
i	Photosynthetic Active Light (PAR) of layer	mol photon $m^{-2}d^{-1}$	A
dz	Height of actual layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myfi2: Light function diatom, n.u.

Equation (3.289) is an analytical solution of the integrated light available for production of flagellates in the water column.

$$myfi2 = (zk2 + \frac{i}{ik2 * eta} * (e^{-eta*zk2} - e^{-eta*dz}))/dz \quad (3.289)$$

Where:

Name	Comment	Unit	Type*)
zk2	Light availability diatom production	m	A
ik2	Light saturation diatome temperature corrected	mol photon $m^{-2}d^{-1}$	A
eta	Vertical light attenuation	m^{-1}	A
i	Photosynthetic Active Light (PAR) of layer	mol photon $m^{-2}d^{-1}$	A
dz	Height of actual layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myfi3: Light function cyanobacteria, n.u.

Equation (3.290) is an analytical solution of the integrated light available for production of flagellates in the water column.

$$myfi3 = (zk3 + \frac{i}{ik3 * eta} * (e^{-eta*zk3} - e^{-eta*dz}))/dz \quad (3.290)$$

Where:

Name	Comment	Unit	Type*)
zk3	Light availability cyanobacteria production	m	A
ik3	Light saturation cyanobacteria temp. corrected	mol photon $m^{-2}d^{-1}$	A
eta	Vertical light attenuation	m^{-1}	A
i	Photosynthetic Active Light (PAR) of layer	mol photon $m^{-2}d^{-1}$	A
dz	Height of actual layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myn1: Nitrogen function flagellates, n.u.

$$myn1 = \frac{PN1/PC1 - pnmi}{(pnma - pnmi)} \tag{3.291}$$

Where:

Name	Comment	Unit	Type*)
PC1	Flagellate phytoplankton C	g C m^{-3}	S
PN1	Flagellate phytoplankton N	g N m^{-3}	S
pnmi	Minimum N:C ratio in phytoplankton	g N g C^{-1}	C
pnma	Maximum N:C ratio in phytoplankton	g N g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myn2: Nitrogen function Diatoms, n.u.

$$myn2 = \frac{\frac{PN2}{PC2} - psmi * pnsi}{(pnma - psmi * pnsi)} \tag{3.292}$$

Where:

Name	Comment	Unit	Type*)
PC2	Diatom phytoplankton C	g C m^{-3}	S
PN2	Diatom phytoplankton N	g N m^{-3}	S
psmi	Minimum Si:C ratio in diatoms	g Si g C^{-1}	C
pnsi	Minimum N:Si ratio in diatoms	g N g Si^{-1}	C
pnma	Maximum N:C ratio in phytoplankton	g N g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myn3: Nitrogen function cyanobacteria, n.u.

$$myn3 = \frac{PN3/PC3 - pnmi}{(pnma - pnmi)} \tag{3.293}$$

Where:

Name	Comment	Unit	Type*)
PC3	Cyanobacteria C	g C m^{-3}	S
PN3	Cyanobacteria N	g N m^{-3}	S
pnmi	Minimum N:C ratio in phytoplankton / cyanobacteria	g N g C^{-1}	C
pnma	Maximum N:C ratio in phytoplankton / cyanobacteria	g N g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myp1: Phosphorous function flagellates, n.u.

$$myp1 = \frac{(kc + ppma - ppmi) * (\frac{PP1}{PC1} - ppmi)}{(ppma - ppmi) * (kc + \frac{PP1}{PC1} - ppmi)} \quad (3.294)$$

Where:

Name	Comment	Unit	Type*)
PC1	Flagellate phytoplankton C	g C m^{-3}	S
PP1	Flagellate phytoplankton P	g P m^{-3}	S
ppmi	Minimum P:C ratio in phytoplankton	g P g C^{-1}	C
ppma	Maximum P:C ratio in phytoplankton	g P g C^{-1}	C
kc	Half saturation concentration for phytoplankton P	g P g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myp2: Phosphorous function diatoms, n.u.

$$myp2 = \frac{(kc + ppma - ppmi) * (\frac{PP2}{PC2} - ppmi)}{(ppma - ppmi) * (kc + \frac{PP2}{PC2} - ppmi)} \quad (3.295)$$

Where:

Name	Comment	Unit	Type*)
PC2	Flagellate phytoplankton C	g C m^{-3}	S
PP2	Flagellate phytoplankton P	g P m^{-3}	S
ppmi	Minimum P:C ratio in phytoplankton	g P g C^{-1}	C

Name	Comment	Unit	Type*)
ppma	Maximum P:C ratio in phytoplankton	g P g C^{-1}	C
kc	Half saturation concentration for phytoplankton P	g P g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myp3: Phosphorous function cyanobacteria, n.u.

$$myp3 = \frac{(\frac{kc}{ppma} * p3pma + p3pma - p3pmi) * (\frac{PP3}{PC3} - p3pmi)}{(p3pma - p3pmi) * (\frac{kc}{ppma} * p3pma + \frac{PP3}{PC3} - p3pmi)} \quad (3.296)$$

Where:

Name	Comment	Unit	Type*)
PC3	Cyanobacteria C	g C m^{-3}	S
PP3	Cyanobacteria P	g P m^{-3}	S
ppmi	Minimum P:C ratio in phytoplankton	g P g C^{-1}	C
ppma	Maximum P:C ratio in phytoplankton	g P g C^{-1}	C
kc	Half saturation conc. for phytoplankton	g P g C^{-1}	C
p3pma	Maximum P:C ratio in cyanobacteria	g P g C^{-1}	C
p3pmi	Minimum P:C ratio in cyanobacteria	g P g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

mys2: Si function, diatoms, n.u

$$mys2 = \frac{\frac{PSi2}{PC2} - psmi}{(psma + psmi)} \quad (3.297)$$

Where:

Name	Comment	Unit	Type*)
PC2	Diatom phytoplankton C	g C m^{-3}	S
PSi2	Diatom phytoplankton Si	g Si m^{-3}	S
psmi	Minimum Si:C ratio in diatoms	g Si g C^{-1}	C
psma	Maximum Si:C ratio in diatoms	g Si g C^{-1}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myte1: Flagellate specific temperature corrected growth, d^{-1}

$$myte1 = mym1 * tet1^{T-20} \quad (3.298)$$

Where:

Name	Comment	Unit	Type*)
mym1	Max. specific net growth at 20 °C, flagellates	d^{-1}	C
tet1	Θ value in Arrhenius relation, flagellate temp. relation	n.u.	C
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myte2: Diatom specific temperature corrected growth, d^{-1}

Smoot_T is a function that makes a smoothing or rolling average of the daily surface insolation (PAR) over a number of days ($T2_{days}$) defined by the user, see auxiliary Smoot_T, Equation (3.318). This smoothing or rolling average is used to adjust the reference temperature of the max. specific growth rate of the diatoms.

The seasonal variation of temperature in the water follow the seasonal variation of the light (PAR) with a delay (1 month) depending of the amount of water (depth) to be heated up. In spring the temperature will be low compared to the daily PAR doze whereas in fall the temperature will be high compared to the daily PAR doze. The diatom reference temperature therefor has to change over the season.

In spring the diatoms blooms at low temperatures and disappear when the silicate is used up. During summer some silicate will be available however the diatom community has changed and another higher reference temperature is needed. In fall a secondary diatom bloom is sometimes seen after the erosion of the pycnocline. The diatom community is again adapted to lower temperatures and decreasing PAR.

Introducing Smoot_T is an attempt to make a seasonal adjustment of the specific growth with the water temperature and light as forcing.

$$myte2 = mym2 * tet2^{T-6-Smoot\_T} \quad (3.299)$$

Where:

Name	Comment	Unit	Type*)
mym2	Max. specific net growth at 6-10 °C, Diatoms	d^{-1}	C
tet2	Θ value in Arrhenius relation, diatom temp. relation	n.u.	C
Smoot_T	Correction of reference temp. for diatoms	°C	A
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

myte3: Cyanobacteria specific temperature corrected growth, d^{-1}

$$myte3 = mym3 * tet3^{T-20} \quad (3.300)$$

Where:

Name	Comment	Unit	Type*)
mym3	Max. specific net growth at 20 °C, cyanobacteria	d^{-1}	C
tet3	Θ value in Arrhenius relation, cyanobacteria temp. relation	n.u.	C
T	Temperature	°C	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

nfix1: Function for N fixation (1 if PSU≤12 else 0), n.u.

$$nfix1 = IF\ S \leq 12\ THEN\ 1\ ELSE\ 0 \quad (3.301)$$

Where:

Name	Comment	Unit	Type*)
S	Salinity	PSU	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

nfix2: Function for N fixation (1 if 0≤PSU≤10 else 0-1), n.u.

$$nfix2 = IF\ S \geq 12\ THEN\ (1 - \frac{S - 10}{12 - 10})\ ELSE\ 1 \tag{3.302}$$

Where:

Name	Comment	Unit	Type*)
S	Salinity	PSU	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

pn1pc1: N:C ration flagellates g N g C^{-1}

$$pn1pc1 = \frac{PN1}{PC1} \tag{3.303}$$

Where:

Name	Comment	Unit	Type*)
PN1	Flagellate phytoplankton N	g N m^{-3}	S
PC1	Flagellate phytoplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

pn2pc2: N:C ration diatomes g N g C^{-1}

$$pn2pc2 = \frac{PN2}{PC2} \tag{3.304}$$

Where:

Name	Comment	Unit	Type*)
PN2	Diatom phytoplankton N	g N m^{-3}	S
PC2	Diatom phytoplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

pn3pc3: N:C ration cyanobacteria g N g C^{-1}

$$pn3pc3 = \frac{PN3}{PC3} \tag{3.305}$$

Where:

Name	Comment	Unit	Type*)
PN3	Cyanobacteria N	g N m^{-3}	S
PC3	Cyanobacteria C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

powNP1: Power function for limiting nutrient, Flagellate (PC1), n.u.

See under auxiliary sed1, Equation (3.18).

powNP3: Power function for limiting nutrient, cyanobacteria (PC3), n.u.

See under auxiliary sed3, Equation (3.29).

pp1pc1: P:C ration flagellates g P g C^{-1}

$$pp1pc1 = \frac{PP1}{PC1} \tag{3.306}$$

Where:

Name	Comment	Unit	Type*)
PP1	Flagellate phytoplankton P	g P m^{-3}	S
PC1	Flagellate phytoplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

pp2pc2: P:C ration diatomes g P g C^{-1}

$$pp2pc2 = \frac{PP2}{PC2} \tag{3.307}$$

Where:

Name	Comment	Unit	Type*)
PP2	Diatom phytoplankton P	g P m^{-3}	S
PC2	Diatom phytoplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

pp3pc3: P:C ration cyanobacteria g P g C^{-1}

$$pp3pc3 = \frac{PP3}{PC3} \tag{3.308}$$

Where:

Name	Comment	Unit	Type*)
PP3	Cyanobacteria P	g P m^{-3}	S
PC3	Cyanobacteria C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

psi2pc2: Si:C ration diatomes g Si g C^{-1}

$$psi2pc2 = \frac{PSi2}{PC2} \tag{3.309}$$

Where:

Name	Comment	Unit	Type*)
PSi2	Diatom Si	g Si m^{-3}	S
PC2	Diatom phytoplankton C	g C m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

rd: Relative daylength, f(month, day,latitude), n.u.

A built in function in ECO Lab that returns a value for relative day length. The value equals 1 at equinox (when day and night have same length).

$$rd = RELATIVE\_DAYLENGTH(\, month, day, latitude) \tag{3.310}$$

sedbouNP1: sedimentation & buoyance N&P function, Flagellate, n.u

Please see auxiliary sed1, Equation (3.18), or buoy1, Equation (3.19)

sedbouNP3: sedimentation & buoyance N&P function, cyanobacteria, n.u

Please see auxiliary sed3, Equation (3.29), or buoy3, Equation (3.30).

sed1: N&P sedimentation function, Flagellate, n.u.

The sedimentation (downward movement) of the algae is increased by low internal N/C and P/C ratios of the algae. powNP1 will be positive but small and sedbuoNP1 becomes negative resulting in a positive value of sed1, see Figure 3.3, under auxiliary buoy1.

$$sed1 = MAX(0, -sedbuoNP1) \tag{3.311}$$

Where:

$$sedbuoNP1 = k2NP * (\frac{powNP1}{powNP1 + k3NP^{k1NP}} - 0.5) \tag{3.312}$$

And:

$$powNP1 = MIN(myp1, myn1)^{k1NP} \tag{3.313}$$

Where:

Name	Comment	Unit	Type*)
k1NP	Exponent, sedimentation& buoyancy, PC1&PC3	n.u.	C
K2NP	Factor for sedimentation & buoyancy, PC1 & PC3	n.u.	C
k3NP	Shift from sedimentation to buoyancy, PC1 & PC3	n.u.	C
powNP1	Power function for limiting nutrient, Flagellate (PC1)	n.u.	A
myn1	Nitrogen function flagellates	n.u.	A
myp1	Phosphorous function flagellates	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

Sed3: N&P sedimentation function, cyanobacteria, n.u.

The sedimentation (downward movement) of the bacteria is increased by low internal N/C and P/C ratios of the bacteria. powNP3 will be positive but small and sedbuoNP3 becomes negative resulting in a positive value of sed3, see Figure 3.4 under auxiliary buou3.

$$sed3 = MAX(0, -sedbuoNP3) \tag{3.314}$$

Where:

$$sedbuoNP3 = k2NP * (\frac{powNP3}{powNP3 + k3NP^{k1NP}} - 0.5) \tag{3.315}$$

And:

$$powNP3 = MIN(myp3, myn3)^{k1NP} \tag{3.316}$$

Where:

Name	Comment	Unit	Type*)
k1NP	Exponent, sedimentation& buoyancy, PC1&PC3	n.u.	C
K2NP	Factor for sedimentation & buoyancy, PC1 & PC3	n.u.	C
k3NP	Shift from sedimentation to buoyancy, PC1 & PC3	n.u.	C
powNP3	Power function for limiting nutrient, cyanobacteria (PC3)	n.u.	A
myn3	Nitrogen function cyanobacteria	n.u.	A
myp3	Phosphorous function cyanobacteria	n.u.	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

SIPm3: PO_4-P in pore water, g P m^{-3}

$$SIPm3 = \frac{SIP}{(1 - dm) * vf * kds} \tag{3.317}$$

Where:

Name	Comment	Unit	Type*)
SIP	Sediment PO_4-P pool	g P m^{-2}	S
dm	Sediment dry matter	g DM gWW^{-1}	C
vf	Sediment bulk density	g ww cm^{-3}	C
Kds	Depth of modelled sediment layer	m	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

Smoot_T: Correction of reference temperature for diatoms, °C

Smoot_T is a function that makes a smoothing or rolling average of the daily insolation (PAR) on surface over a number of days ($T2_{days}$) defined by the user. This smoothing or rolling average is used to adjust the reference temperature of the max. specific growth rate of the diatoms, see auxiliary *myte2,* Equation (3.299).

The seasonal variation of temperature in the water follow the seasonal variation of the light (PAR) with a delay (1 month) depending of the amount of water (depth) to be heated up. In spring the temperature will be low compared to the daily PAR doze whereas in fall the temperature will be high compared to the daily PAR doze. The diatom reference temperature therefor has to change over the season.

In spring the diatoms blooms at low temperatures and disappear when the silicate is used up. During summer some silicate will be available however the diatom community has changed and another higher reference temperature is needed. In fall a secondary diatom bloom is sometimes seen after the erosion of the pycnocline. The diatom community is again adapted to lower temperatures and decreasing PAR.

Introducing Smoot_T is an attempt to make a seasonal adjustment of the specific growth with the water temperature and light as forcing.

One of two builtin functions can be used SMOOTING_AVERAGE or MOVING_AVERAGE can be used, see (MIKE by DHI 2011b). The latter function demands more memory and increases the CPU time slightly.

$$Smoot\_T = \frac{difT2}{maxI_0} * SMOOTHING\_AVERAGE(i_0, \frac{DT_{day}}{T2_{days}}) \quad (3.318)$$

Where:

Name	Comment	Unit	Type*)
difT2	Max variation in reference temp., diatom production	°C	C
$maxI_0$	Max average monthly i_o of year (July or Jan.)	mol photon $m^{-2}d^{-1}$	C
i_0	Light (PAR) at surface	mol photon $m^{-2}d^{-1}$	F
DT_{day}	AD time step in days, (normally between 5 min. to 1 h)	d	F
$T2_{days}$	No. of days in smoothing or rolling average function	d	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

SNHm3: NH4-N in sediment pore water, g N m^{-3}

$$SNHm3 = \frac{SNH}{(1 - dm) * vf * kds} \quad (3.319)$$

Where:

Name	Comment	Unit	Type*)
SNH	Sediment NH_4-N pool	g N m^{-2}	S
dm	Sediment dry matter	g DM gWW^{-1}	C
vf	Sediment bulk density	g ww cm^{-3}	C
Kds	Depth of modelled sediment layer	m	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

SNO3m3: NO_3-N in pore water of surface sediment layer (0-KDO2) , g N m^{-3}

$$SNO3m3 = \frac{SNO3}{(1 - dm) * vf * KDO2} \quad (3.320)$$

Where:

Name	Comment	Unit	Type*)
SNO3	Sediment NO_3-N pool	g N m^{-2}	S
dm	Sediment dry matter	g DM gWW^{-1}	C
vf	Sediment bulk density	g ww cm^{-3}	C
KDO2	Depth of O_2 penetration in sediment	m	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

sqdo: Oxygen function, n.u.

$$sqdo = \frac{DO^{ndo3}}{DO^{ndo3} + mdo3} \tag{3.321}$$

Where:

Name	Comment	Unit	Type*)
DO	Oxygen	g O_2 m^{-3}	S
ndo3	Exponent for DO in sqdo	n.u.	C
mdo3	Half-saturation constant DO	g O_2 m^{-3}	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

zk1: Light penetration (availability) in actual layer for flagellate production, m

$$zk1 = MIN(dz, MAX(0, \frac{\ln(i) - \ln(ik1)}{eta})) \tag{3.322}$$

Where:

Name	Comment	Unit	Type*)
i	Light (PAR) in actual layer	mol photon $m^{-2}d^{-1}$	A
ik1	Light saturation temp. corrected, Flagellate	mol photon $m^{-2}d^{-1}$	A
eta	Vertical light extinction in layer	m^{-1}	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

zk2: Light penetration (availability) in actual layer for diatom production, m

$$zk1 = MIN(dz, MAX(0, \frac{\ln(i) - \ln(ik2)}{eta})) \tag{3.323}$$

Where:

Name	Comment	Unit	Type*)
i	Light (PAR) in actual layer	mol photon $m^{-2}d^{-1}$	A
lk2	Light saturation temp. corrected, diatoms	mol photon $m^{-2}d^{-1}$	A
eta	Vertical light extinction in layer	m^{-1}	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

zk3: Light penetration (availability) in actual layer for cyanobacteria production, m

$$zk1 = MIN(dz, MAX(0, \frac{\ln(i) - \ln(ik3)}{eta})) \quad (3.324)$$

Where:

Name	Comment	Unit	Type*)
i	Light (PAR) in actual layer	mol photon $m^{-2}d^{-1}$	A
lk3	Light saturation temp. corrected, cyanobacteria	mol photon $m^{-2}d^{-1}$	A
eta	Vertical light extinction in layer	m^{-1}	A
dz	Height of actual water layer	m	F

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

unh1: potential NH_4 uptake by flagellates, g N m^{-3} d^{-1}

$$unh1 = PC1 * maxupnh * \frac{NH4}{NH4 + hupnh} \quad (3.325)$$

Where:

Name	Comment	Unit	Type*)
PC1	Flagellate C	g C m^{-3}	S
maxupnh	Max. N uptake by phytoplankton during N limitation	g N g $C^{-1}d^{-1}$	C
hupnh	Half-saturation constant for NH_4, phytoplankton uptake	g N m^{-3}	C
NH4	NH_4-N in water	g N m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

unh2: potential NH_4 uptake by diatoms, g N m^{-3} d^{-1}

$$unh2 = PC2 * pda2 * maxupnh * \frac{NH4}{NH4 + hupnh * pdb2} \quad (3.326)$$

Where:

$$pda2 = (\frac{esd2}{esd1})^{kbt1} \quad (3.327)$$

And:

$$pdb2 = (\frac{esd2}{esd1})^{kbt2} \quad (3.328)$$

Where:

Name	Comment	Unit	Type*)
PC2	Diatom C	g C m^{-3}	S
maxupnh	Max. N uptake by flagellates during N limitation	g N g $C^{-1}d^{-1}$	C
hupnh	Half-saturation constant for NH_4, phytoplankton uptake	g N m^{-3}	C
NH4	NH_4-N in water	g N m^{-3}	S
pda2	Ratio, nutrient uptake, Diatom : Flagellate	n.u.	A
pdb2	Ratio, half saturation conc. Diatom: Flagellate	n.u.	A
esd1	Equivalent spherical diameter, flagellates	µm	C

Name	Comment	Unit	Type*)
esd2	Equivalent spherical diameter, Diatom	µm	C
kbet1	Exponent 1 for potential uptake of nutrients	n.u.	C
kbet2	Exponent 2 for half saturation conc.	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

unh3: Potential NH4 uptake by cyanobacteria, g N m^{-3} d^{-1}

$$unh3 = PC3 * pda3 * maxupnh * \frac{NH4}{NH4 + hupnh * pdb3} \quad (3.329)$$

Where:

$$pda3 = (\frac{esd3}{esd1})^{kbt1} \quad (3.330)$$

And:

$$pdb3 = (\frac{esd3}{esd1})^{kbt2} \quad (3.331)$$

Where:

Name	Comment	Unit	Type*)
PC3	Cyanobacteria C	g C m^{-3}	S
maxupnh	Max. N uptake by flagellates during N limitation	g N g $C^{-1}d^{-1}$	C
hupnh	Half-saturation constant for NH_4, phytoplankton uptake	g N m^{-3}	C
NH4	NH_4-N in water	g N m^{-3}	S
pda3	Ratio, nutrient uptake, Cyanobacteria : Flagellate	n.u.	A
pdb3	Ratio, half saturation conc. Cyanobacteria: Flagellate	n.u.	A
esd1	Equivalent spherical diameter, flagellates	µm	C
esd3	Equivalent spherical diameter, Cyanobacteria	µm	C
kbet1	Exponent 1 for potential uptake of nutrients	n.u.	C
kbet2	Exponent 2 for half saturation conc.	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

un31: Potential NO_3 uptake by flagellate, g N m^{-3} d^{-1}

$$un31 = PC1 * maxupn3 * \frac{NO3}{NO3 + hupn3} \quad (3.332)$$

Where:

Name	Comment	Unit	Type*)
PC1	Flagellate C	g C m-3	S
maxupn3	Max. NO3 uptake by phytoplankton during N limitation	g N g $C^{-1}d^{-1}$	C
hupnh3	Half-saturation constant for NO3, phytoplankton uptake	g N m^{-3}	C
NO3	NO3-N in water	g N m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

un32: Potential NO_3 uptake by diatoms, g N m^{-3} d^{-1}

$$un32 = PC2 * pda2 * maxupn3 * \frac{NO3}{NO3 + hupn3 * pdb2} \quad (3.333)$$

Where:

$$pda2 = (\frac{esd2}{esd1})^{kbt1} \quad (3.334)$$

And:

$$pdb2 = (\frac{esd2}{esd1})^{kbt2} \quad (3.335)$$

Where:

Name	Comment	Unit	Type*)
PC2	Diatom C	g C m^{-3}	S
maxupn3	Max. NO_3 uptake by flagellates during N limitation	g N g $C^{-1}d^{-1}$	C
hupn3	Half-saturation constant for NO_3, phytoplankton uptake	g N m^{-3}	C
NO3	NO_3-N in water	g N m^{-3}	S
pda2	Ratio, nutrient uptake, Diatom : Flagellate	n.u.	A
pdb2	Ratio, half saturation conc. Diatom: Flagellate	n.u.	A
esd1	Equivalent spherical diameter, flagellates	µm	C
esd2	Equivalent spherical diameter, Diatom	µm	C

Name	Comment	Unit	Type*)
kbet1	Exponent 1 for potential uptake of nutrients	n.u.	C
kbet2	Exponent 2 for half saturation conc.	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

un33: Potential NH_4 uptake by cyanobacteria, g N m^{-3} d^{-1}

$$un33 = PC3 * pda3 * maxupn3 * \frac{NO3}{NO3 + hupn3 * pdb3} \quad (3.336)$$

Where:

And:

$$pda3 = (\frac{esd3}{esd1})^{kbt1} \quad (3.337)$$

$$pdb3 = (\frac{esd3}{esd1})^{kbt2} \quad (3.338)$$

Where:

Name	Comment	Unit	Type*)
PC3	Cyanobacteria C	g C m^{-3}	S
maxupn3	Max. NO_3 uptake by flagellates during N limitation	g N g $C^{-1}d^{-1}$	C
Hupn3	Half-saturation constant for NO_3, phytoplankton uptake	g N m^{-3}	C
NO3	NO_3-N in water	g N m^{-3}	S
pda3	Ratio, nutrient uptake, Cyanobacteria : Flagellate	n.u.	A
pdb3	Ratio, half saturation conc. Cyanobacteria: Flagellate	n.u.	A
esd1	Equivalent spherical diameter, flagellates	µm	C
esd3	Equivalent spherical diameter, Cyanobacteria	µm	C
kbet1	Exponent 1 for potential uptake of nutrients	n.u.	C
kbet2	Exponent 2 for half saturation conc.	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

upo1: Potential PO_4 uptake by flagellate, g P m^{-3} d^{-1}

$$upo1 = PC1 * maxupip * \frac{PO4}{PO4 + hupp} \quad (3.339)$$

Where:

Name	Comment	Unit	Type*)
PC1	Flagellate C	g C m^{-3}	S
maxupip	Max. P uptake by phytoplankton during P limitation	g P g $C^{-1}d^{-1}$	C
hupip	Half-saturation constant for PO_4, phytoplankton uptake	g P m^{-3}	C
PO4	PO_4-P in water	g P m^{-3}	S

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

upo2: Potential PO_4 uptake by diatoms, g P m^{-3} d^{-1}

$$upo2 = PC2 * pda2 * maxupip * \frac{PO4}{PO4 + hupp * pdb2} \quad (3.340)$$

Where:

$$pda2 = (\frac{esd2}{esd1})^{kbt1} \quad (3.341)$$

And:

$$pdb2 = (\frac{esd2}{esd1})^{kbt2} \quad (3.342)$$

Where:

Name	Comment	Unit	Type*)
PC2	Diatom C	g C m^{-3}	S
maxupip	Max. PO_4 uptake by flagellates during P limitation	g P g $C^{-1}d^{-1}$	C
hupp	Half-saturation constant for PO_4, phytoplankton uptake	g P m^{-3}	C
PO4	PO_4-P in water	g P m^{-3}	S
pda2	Ratio, nutrient uptake, Diatom : Flagellate	n.u.	A
pdb2	Ratio, half saturation conc. Diatom: Flagellate	n.u.	A
esd1	Equivalent spherical diameter, flagellates	µm	C

Name	Comment	Unit	Type*)
esd2	Equivalent spherical diameter, Diatom	µm	C
kbet1	Exponent 1 for potential uptake of nutrients	n.u.	C
kbet2	Exponent 2 for half saturation conc.	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

upo3: Potential PO_4 uptake by cyanobacteria, g P m^{-3} d^{-1}

$$upo3 = PC3 * pda3 * maxupip * \frac{PO4}{PO4 + hupp * pdb3} \quad (3.343)$$

Where:

$$pda3 = (\frac{esd3}{esd1})^{kbt1} \quad (3.344)$$

And:

$$pdb3 = (\frac{esd3}{esd1})^{kbt2} \quad (3.345)$$

Where:

Name	Comment	Unit	Type*)
PC3	Cyanobacteria C	g C m^{-3}	S
maxupip	Max. PO_4 uptake by flagellates during P limitation	g P g $C^{-1}d^{-1}$	C
hupp	Half-saturation constant for PO_4, phytoplankton uptake	g P m^{-3}	C
PO4	PO_4-P in water	g P m^{-3}	S
pda3	Ratio, nutrient uptake, Cyanobacteria : Flagellate	n.u.	A
pdb3	Ratio, half saturation conc. Cyanobacteria: Flagellate	n.u.	A
esd1	Equivalent spherical diameter, flagellates	µm	C
esd3	Equivalent spherical diameter, Cyanobacteria	µm	C
kbet1	Exponent 1 for potential uptake of nutrients	n.u.	C
kbet2	Exponent 2 for half saturation conc.	n.u.	C

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

usi2: Potential Si uptake by diatoms, g Si m^{-3} d^{-1}

$$usi2 = PC2 * maxupsi * \frac{Six}{Six + hupsi} \quad (3.346)$$

Where:

$$six = Si - Simin \quad (3.347)$$

Where:

Name	Comment	Unit	Type*)
PC2	Flagellate C	g C m^{-3}	S
maxupsi	Max. Si uptake by phytoplankton during Si limitation	g Si g $C^{-1}d^{-1}$	C
hupsi	Half-saturation constant for Si, diatom uptake	g Si m^{-3}	C
Six	available Si for diatoms, (Si-Simin) >=0, Si for uptake PC2	g Si m^{-3}	A
Si	Si in water	g Si m^{-3}	S
Simin	Si not available for PC2	g Si m^{-3}	A

*) S: State variable, F: Forcing, C: Constant, P: Process in differential equation, P1: Help process, A: Auxiliary help process.

4 Data Requirements

- Basic Model Parameters
  - Model grid size and extent
  - Time step and length of simulation
  - Type of output required and its frequency
- Bathymetry and Hydrodynamic Input
- Combined Advection-Dispersion Model
  - Dispersion coefficients
- Initial Conditions
  - Concentration of parameters
- Boundary Conditions
  - Concentration of parameters
- Pollution Sources
  - Discharge magnitudes and concentration of parameters
- Process Rates
  - Size of coefficients governing the process rates. Some of these coefficients can be determined by calibration. Others will be based on literature values or found from actual measurements and laboratory tests.
- Forcings
- Data sets of photosynthetic active light (PAR) ($E/m^2/day$)

5 References

/1/ Droop M.R. 1973. Some thoughts on nutrient limitation in algae. J. Phycol. 9 P:264-272.

/2/ Droop M.R. 1975. The nutrient status of algae cells in bach cultures. J. Mar. Biol. Ass. U.K. 55 P:541-555.

/3/ Effer S.W. 1988. Secchi disk transparency and turbidity. Journal of environmental engineer-ing. 1988 vol. 114 no. 6 pp. 1436-1447.

/4/ Kirk J.T.O. 2000. Light and photosynthesis in aquatic ecosystems. Cambridge University Press 2. Edition 2000. ISBN 0521453534, ISBN 052145459664

/5/ Lund-Hansen L.C. 2004. Diffuse attenuation coefficients Kd(PAR) at estuarine North Sea-Baltic Sea transition: time-series, partitioning, absorption, and scattering. Estuarine, Coastal and Shelf Science 61 (2004) pp:251-259.

/6/ MIKE by DHI 2011a. MIKE 21 & MIKE 3 Flow Model. Mud Transport module Scientific Description. DHI water environment health, Hørsholm Denmark

/7/ MIKE by DHI 2011b. ECO Lab User guide. DHI water environment health, Hørsholm Denmark

/8/ Monod J. 1949. The Growth of Bacterial Cultures. Annual Review of Microbiology, v. 3, p. 371.

/9/ Morel A. 1980. In water and remote measurements of ocean color. Boundary-Layer Meteor-ology 18 (1980) pp 177-201.

/10/ Nyholm N. 1977 Kinetics of phosphate-limited algae growth. Biotechn. Bioengineering 19 P:467-492.

/11/ Nyholm N. 1978 A simulation model for phytoplankton growth cycling in eutrophic shallow lakes. Ecological Modelling. Vol. 4, P:279-310.

/12/ Nyholm N. 1979 The use of management models for lakes at the Water Quality Institute. Denmark. Ste –of-the-art in Ecological Modelling. Vol. 7. P:561-577.

/13/ Pfannkuche F. 2002. Optical properties of Otago Shelf Waters: South Island New Zealand. Estuarine, Coastal and Shelf Science 55 (2002) pp:613-627.

/14/ Prieur L., S. Sathyendranath 1981. An optical classification of coastal and oceanic waters based on the specific spectral absorption curves of phytoplankton pigments, dissolved or-ganic matter, and other particulate materials. Limnol. Oceanogr. 26(4) PP 671-689.

/15/ Rasmussen Erik Kock, O.S. Petersen, J.R. Thomsen, R. J. Flower, F. Aysche, M. Kraiem, L. Chouba 2009. Model analysis of the future water quaity of the eutrophicated Ghar EL Melh lagoon (Northern Tunesia). Hydrobiologia (2009) 622:173-193

/16/ Tett P., A. Edvards & K. Jones 1986. A model for the growth of shelf-sea phytoplankton in summer. Estuar. Coast. Shelf Sci. 23 P:641-672.

MIKE
Powered by DHI

ECO Lab

Short Scientific Description

PLEASE NOTE

PRINTING HISTORY

November 2003
June 2004
April 2006
...
September 2012
October 2013
July 2015

CONTENTS

1 Introduction

ECO Lab is a piece of numerical simulation software for Ecological Modelling developed by DHI. It is an open and generic tool for customising aquatic ecosystem models to simulate for instance water quality, eutrophication, heavy metals and ecology.

ECO Lab functions as a module in the MIKE simulation software.

The module is developed to describe processes and interactions between chemical and ecosystem state variables. Also the physical process of sedimentation of state variables can be described (moves the state variable physically down the water column).

The module is coupled to the Advection-Dispersion Modules of the DHI hydrodynamic flow models, so that transport mechanisms based on advection-dispersion can be integrated in the ECO Lab simulation.

The description of the ecosystem state variables in ECO Lab is formulated as a set of ordinary coupled differential equations describing the rate of change for each state variable based on processes taking place in the ecosystem. All information about ECO Lab state variables, processes and their interaction are stored in a so-called generic ECO Lab template.

2 What Is Behind ECO Lab?

ECO Lab uses a so-called ECO Lab COM[1] object to perform the ECO Lab calculations. The ECO Lab object is generic and shared with a number of different DHI flow model systems. It consists of an interpreter that first translates the equation expressions in the ECO Lab template[2] to lists of instructions that enables the object to evaluate all the expressions in the template. During simulation the model system integrates one time step by simulating the transport of advective state variables based on hydrodynamics. Initial concentrations or updated AD concentrations, coefficients/constants and updated forcing functions are loaded into the ECO Lab object and then the ECO Lab object evaluates all the expressions, integrates one time step, and returns updated concentration values to the general flow model system that advances one time step. An illustration of the data flow is shown in Figure 2.1.

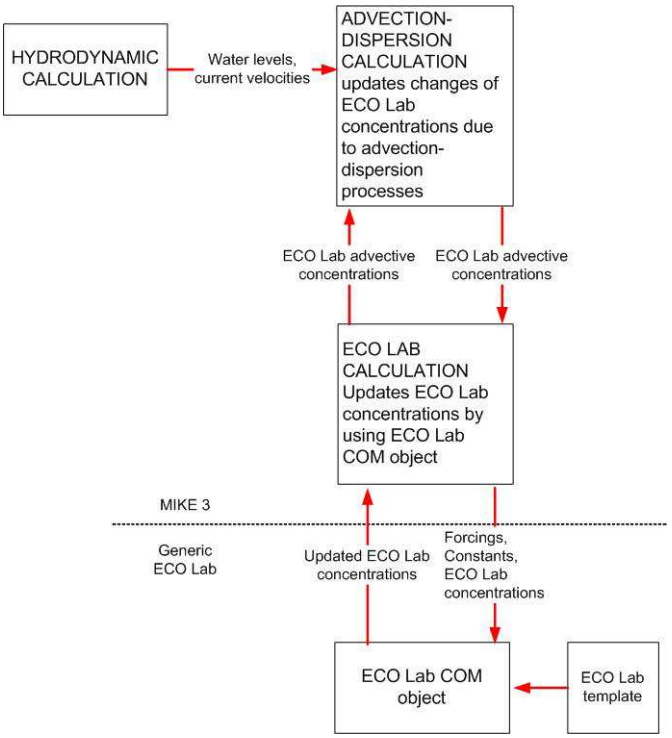

Figure 2.1 Data flow between the hydrodynamic flow model, in this case MIKE 3, and ECO Lab.

1 Microsoft COM standard
2 An ECO Lab template contains the mathematical definition of an ECO Lab model. It contains information about the included state variables, constants, forcings, processes and the state variables' rate-of-change differential equations.

3 ECO Lab Set of Ordinary Differential Equations

In general an ordinary differential equation is specified for each state variable.

The ordinary differential equation summaries the processes involved for the specific state variable. If a process affect more than one state variable, or the state variables affect each other, the differential equations are said to be coupled with each other.

The processes contain mathematical expressions using arguments such as numbers, constants, forcings and state variables. Processes always describe the rate at which something changes. In this context constants are values always constant in time, and forcings are values that can be varying in time.

$$P_c = \frac{dc}{dt} = \sum_{i=1}^{n} process_i \qquad (3.1)$$

c: The concentration of the ECO Lab state variable

n: Number of processes involved for specific state variable

The Unit for 'Rate of change' of P_c can be specified as 3 types:

- $g/m^2/d$
- mg/l/d
- Undefined

In general the part of the unit that relates to time shall always be specified as 'per day' in the template.

In ECO Lab there are two kinds of processes: transformation and settling processes. Transformation is a point description of a process not dependent on neighbouring points. Settling is a process transporting state variables to neighbouring points down the water column. The calculation of a state variable with a settling process is therefore dependent on information from neighbouring points. Also, the light forcing needs special handling to calculate the light penetration in the water column. A special built-in function can be used for this purpose. ECO Lab can also handle that some processes only take place at specific positions in the water column. For instance should reaeration (exchange with the atmosphere) only take place in the water surface. In other parts of the water column the reaeration is not active.

3.1 Special handling of settling process

The calculation of vertical movements need information from the layer below or above in multi layered systems. It is possible to in ECO Lab to specify one type of process with vertical movement: settling. This process is transporting the state variable vertically towards the bottom. As for transformation processes an expression must be specified describing the 'concentration change' from actual cell to cell below [mg/l/d]. When looking at a 'Settling' process directly in output from an ECO Lab simulation the output will show the result of the specified expression (the same as if it was a transformation process). The difference between a 'Settling' and a 'Transformation' process will appear in output of the affected state variable. This is because the numerical solution of a state variable affected by a 'Settling' process is different than if it was a 'Transformation' process. The definition of sign for a settling process is so that it should be specified as minus in the differential equation in order to transport the state variable correctly down the water column. The solution of a state variable with a settling process in a multilayered system takes into account that a contribution to the state variable is received from the layer above (if not top layer). Any variation in vertical discretization is also included in the numerical solution of differential equation involving a settling process. When solving a differential equation containing a settling process, ECO Lab substitutes the settling process expression in the differential equation with the following expression;

$$\frac{dc_n}{dt} = \frac{-settling_{n-1} \cdot dz_{n-1} + settling_n \cdot dz_n}{dz_n} \tag{3.2}$$

where

- $settling_{n-1}$ is the userspecified expression for 'rate of change' of the state variable concentration in layer n caused by a settling process transporting from layer n-1 to layer n [g·m-3·d-1]. It is usually a function of the concentration in layer n -1.
- $settling_n$ is the userspecified expression for 'rate of change' of the state variable concentration in layer n caused by a settling process transporting from layer n to layer n+1 [g·m-3·d-1]. It is usually a function of the concentration in layer n.
- dz_n is the thickness of layer *n* [m] and dz_{n-1} is the thickness of layer *n*–1 [m].

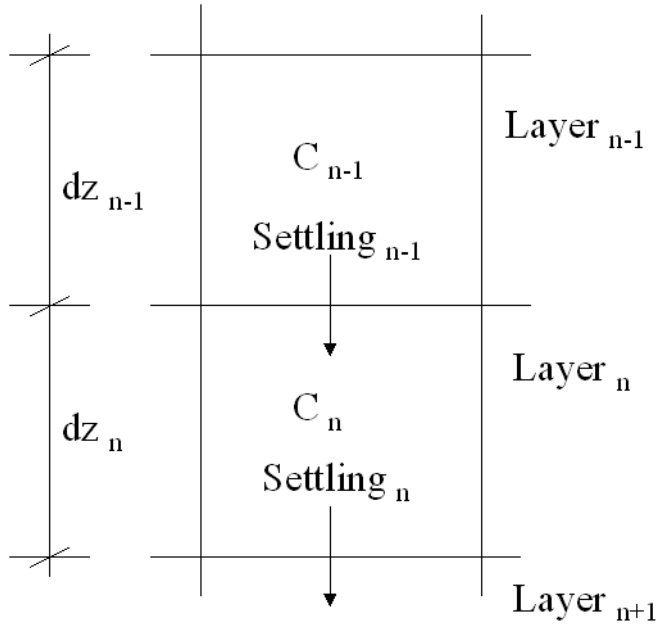

Figure 3.1 Schematic illustration of settling process

3.2 Special handling of light penetration in ECO Lab

Light penetration in the water column can be solved with a Lambert Beer built-in function in ECO Lab. In multi-layered systems with vertical varying extinction coefficients, the Lambert Beer expression must be calculated for each layer, and therefore, the Lambert Beer expression as argument uses the result of the Lambert Beer expression in the layer above.

$$I_n = I_{n-1} \cdot e^{\pi_n \cdot dz_n} \tag{3.3}$$

where I_n is the light available for primary production in the actual layer *n,* I_{n-1} is the irradiance in the layer above, η_n is the extinction coefficient and dz_n the layer thickness.

The way ECO Lab handles this problem is by using a so-called built-in function that is special designed to handle this 'Lambert Beer' problem. The functions are called:

- LAMBERT_BEER_1(surface radiation, layer height, light extinction coefficient). The function returns the solar radiation in top of each layer of the water column.
- LAMBERT_BEER_2(surface radiation, layer height, light extinction coefficient). The function returns the solar radiation in bottom of each layer of the water column.

3.3 Handling of built-in constants and forcings

Forcings such as for instance temperature can be specified in different ways. They can be user specified, as constant values or as timeseries, map series, or volume series. As an alternative to using user specified values of constants and forcings, it is also possible to use built-in forcing and constants. Built-in constants and forcings can be picked from a list in the dialog and they are already estimated in the hydrodynamic model, and they can be used as arguments in ECO Lab expressions. During simulation the built-in forcings and constants will be updated with the calculations in the hydrodynamic simulation. Examples of built-in forcings are temperature, flow velocities, salinity, wind velocity.

3.4 Handling of site specific processes

Some processes only take place in specific layers of the water column, and such processes are handled by calculating the process at the relevant layer where the process takes place and setting the process to zero in other layers. Examples of this could be a process such as re-aeration.

3.5 Example of ordinary ECO Lab differential equation:

Cyanide is assumed only to be affected by one temperature dependent decay process in this simple example;

$$\frac{dc_{cyanide}}{dt} = -decay$$

$$decay = K \cdot \Theta^{(temperature - 20)} \cdot c_{cyanide}$$

K: Decay coefficient (day^{-1})

Θ: Arrhenius temperature coefficient

The scientific descriptions of specific ECO Lab differential equations and process equations in DHI supported ECO Lab templates has a PDF file attached containing scientific description of the template in question. For DHI projects with tailor-made ECO Lab templates for specific projects, the scientific description of the used ECO Lab equations typically will be described in the project report.

4 Integration With AD Engines

The dynamics of advective ECO Lab state variables can be expressed by a set of transport equations, which in non-conservative form can be written as:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = D_x\frac{\partial^2 c}{\partial z^2} + D_y\frac{\partial^2 c}{\partial z^2} + D_z\frac{\partial^2 c}{\partial z^2} + S_c + P_c \quad (4.1)$$

c:	The concentration of the ECO Lab state variable
u, v, w:	Flow velocity components
Dx, Dy, Dz:	Dispersion coefficients
Sc:	Sources and sinks
Pc:	ECO Lab processes

The state variables may be coupled linearly or non-linearly to each other through the ECO Lab source term P_c

The transport equation can be rewritten as

$$\frac{\partial c}{\partial t} = AD_c + P_c \quad (4.2)$$

where the term AD_c represents the rate of change in concentration due to advection, dispersion (including sources and sinks).

The ECO lab numerical equation solver makes an explicit time-integration of the above transport equations, when calculating the concentrations to the next time step.

An approximate solution is obtained in ECO Lab by treating the advection-dispersion term as AD_c as constant in each time step.

The coupled set of ordinary differential equations defined in ECO Lab are solved by integrating the rate of change due to both the ECO Lab processes themselves and the advection-dispersion processes.

$$c(t+\Delta t) = \int_t^{t+\Delta t} (P_c(t) + AD_c) + \partial t \quad (4.3)$$

The advection-dispersion contribution is approximated by

$$AD_c = \frac{c^* + (t + \Delta t) - c^n(t)}{\Delta t} \tag{4.4}$$

where the intermediate concentration c* is found by transporting the ECO Lab state variable as a conservative substance over the time period Δt using the AD module.

The main advantage of this approach is that the explicit approach resolve coupling and non-linearity problems resulting from complex source ECO Lab terms P_c, and therefore the ECO Lab and the advection-dispersion part can be treated separately.

An implicit approach of solving the transport equations is not possible yet in ECO Lab.

5 Integration Methods

The following integration methods are available in ECO Lab: Euler, Runge Kutta 4, Runge Kutta with quality check.

5.1 Euler integration method

A very simple numerical solution method for solving ordinary differential equations.

The formula for the Euler method is:

$$y_{n+1} = y_n + h \cdot f(x_n, y_n) \tag{5.1}$$

which advances a solution y from x_n to $x_{n+1} = x_n + h$

5.2 Runge Kutta 4th order

A classical numerical solution method for solving ordinary differential equations. It has usually higher accuracy than the Euler method, but requires longer simulation times. The fourth order Runge-Kutta method requires four evaluations of the right hand side per time step.

$$y_{n+1} = \mathrm{rk4}(y_n, f(x_n, y_n), x_n, h) \tag{5.2}$$

The function is solved this way:

$$k_1 = h \cdot f(x_n, y_n) \tag{5.3}$$

$$k_2 = h \cdot f\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$

$$k_3 = h \cdot f\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right)$$

$$k_4 = h \cdot f(x_n + h, y_n + k_3)$$

$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} - O(h^5)$$

which advances a solution y from x_n to $x_{n+1} = x_n + h$

5.3 Runge Kutta 5th order with quality check

A numerical solution method for solving ordinary differential equations. The accuracy is evaluated and the time step is adjusted if results are not accurate enough.

$$y_{n+1} = f(y_n, f(y_n, x_n),\ x_n, h, \varepsilon, \text{yscale}) \tag{5.4}$$

The function is solved this way:

First take two half steps:

$$h_2 = 0.5 \cdot h \tag{5.5}$$

$$x_{n+½} = x_n + h_2 \tag{5.6}$$

$$y_2 = \text{rk4}(y_n, f(y_n, x_n),\ x_n, h_2) \tag{5.7}$$

$$y_2 = \text{rk4}(y_2, f(y_2, x_{n+½}),\ x_{n+½}, h_2) \tag{5.8}$$

Compare with one full time step:

$$y_1 = \text{rk4}(y_n, f(y_n, x_n),\ x_n, h) \tag{5.9}$$

Then estimate error:

$$y_1 = y_2 - y_1 \tag{5.10}$$

$$\text{err} = \text{MAX}(\text{ABS}(y_1/\text{yscale}))/\varepsilon \tag{5.11}$$

If the error is small (err <= 1.0) the function returns

$$y_{n+1} = y_2 + \frac{y_1}{15} \tag{5.12}$$

which advances a solution y from x_n to $x_{n+1} = x_n + h$

or else the time step is reduced and the function tries again.

Answers to expert panel based on "questions from the panel to the researchers" made available to the researchers from 16/8-2017 through an e-mail from Implement.

General questions

Exclusive focus on reducing land-based N load to obtain good ecological status

Both the panel and the stakeholders miss a justification of the fundamental choice to focus exclusively on reduction of (diffuse) N sources as the main means to improve water quality.

Comment: We did not choose to focus exclusively on N reductions. The focus on nitrogen was a consequence of the agreement with the authorities to focus on the intercalibrated quality element indicators summer chlorophyll-and eelgrass depth limit (the latter described by the proxy-indicator K_d). Both the statistical and mechanistic models include N and P as well as several climatic factors known to affect the parameters chlorophyll-a and K_d. However, the modelling work showed that these included indicators were most sensitive towards nitrogen reductions whereas reductions in phosphorous did not significantly affect the indictors. Hence, we cannot document that phosphorous reductions will affect the indicators – whereas we can document that nitrogen reductions will. Currently, a research project is trying to identify P-sensitive indicators that could be included in a more holistic assessment of marine water quality.

The situation is complex, as there is ample evidence that in many systems there is co-limitation of phytoplankton growth by N and P, with some seasonal pattern in most systems.

Comment: We agree, and we observe this seasonality in most estuaries and coastal Danish marine waters as well, with P limitation in spring and N limitation during summer/autumn. This seasonality in N versus P limitation in DK waters, and especially N limitation during summer, is supported by several studies (Hansen 2016), (Timmermann et al., 2010), (Carstensen et al., 2007), (Pedersen 1995), (Nielsen et al., 2002b), (Møhlenberg et al., 2007). Although, we fully recognize the importance of P for water quality (in a broad sense), we could not document P sensitivity for the applied indicators in most Danish water bodies covered by the developed models.

In addition, N fixation in the Baltic may aggravate the problem and undo N reduction measures where ample P is available. But it is also true that the N:P ratio of winter loadings is biased towards N, and that historical reductions have affected P loadings much more than N loadings.

Comment: Large occurrences of cyanobacteria in Danish waters are rare and limited to the southern part of Øresund/western Baltic Sea properly due to the high salinity (>10 psu). Figure 1 (from Lyngsgaard PhD thesis 2013) shows the contribution of cyanobacteria and other phytoplankton groups at three sites

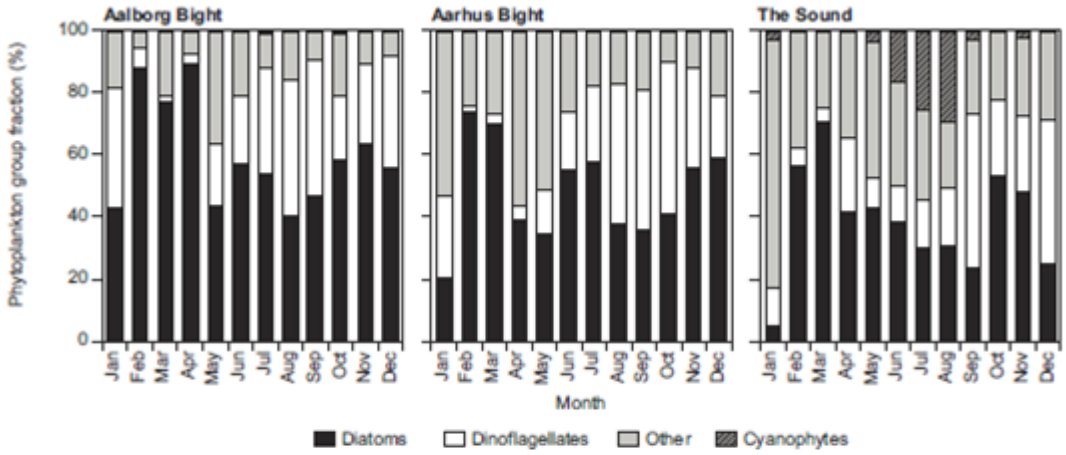

Figure 8. Average monthly percentage distribution of the following phytoplankton groups; Diatoms, Dinoflagellates, Cyanophytes and 'Other' (including the remaining phytoplankton groups), for the euphotic zone at three locations in the BSTZ.

The figure show that cyanobacteria only occur in measureable numbers in The Sound in June to August. These occurrences (mean over decades) reflect that cyanobacteria irregularly flow into the south-eastern part of the Danish waters from the Baltic Sea. Although they can represent a significant problem for water quality, the population is decaying and the N-fixation rates are low or absent as they are not growing.

As cyanobacteria only may occur in a few Danish water bodies N fixation in Danish waters is neghlegtable as N source (Jorgensen et al., 2014) and in-situ N fixation in DK waters is not likely to counteract any future N load reduction. In the central Baltic Sea, N fixation is, however, an important N source, which potentially may result in increased TN concentration in the central Baltic Sea and consequently impact especially the more open part of the Danish water bodies, and thus potentially counteract (some of) the N reduction efforts from Danish catchments for these areas. It is, however, a prerequisite for the performed scenarios and following reduction targets that the BSAP have been implemented, and this plan is expected to reduce the problem with cyanobacteria in the central Baltic Sea over time. For water bodies dominated by Danish catchments, and less affected by Baltic Sea water, riverine concentrations of bioavailable TN is generally 25-30 times higher than in Baltic Sea waters and hence slightly increased Baltic Sea TN concentrations is not likely to influence the environmental conditions of most Danish estuaries.

Questions and answers

Q: We are in need of a thorough literature-based justification of the choices made, as this is a key aspect of the whole study and the policy.

A: As mentioned above, focus on N reduction was not a choice per se, but an emergent property when focusing on the indicators pre-determined to be the focus of the performed study. Whether N and/or P is limiting primary production and act as bottom up control of phytoplankton biomass varies with location and season (Tamminen and Andersen 2007; Hrustic et al., 2017; Burson et al., 2016). In Danish marine waters, P is often found to be limiting in the spring whereas N becomes limiting during late spring/early summer and remains the limiting nutrient (Hansen 2016; Timmermann et al., 2010; Carstensen et al., 2007; Pedersen 1995; Nielsen et al., 2002b) and also the results from the present study show that N loading (and not P loading) is controlling the addressed indicators in the dominant part of the examined water bodies. It must be noticed that in the statistical as well as the mechanistic model approach, both N and P input are

included (from Danish catchment: both approaches and from atmosphere, sediment and via exchange with North Sea and Baltic Sea: mechanistic model approach). Furthermore several climatic parameters known to influence the indicators directly (e.g.light) or indirectly (e.g. via influence on water temperature and hydrodynamic properties) are included. The choice of including N and P as potential controlling factors is based on a vast amount of literature documenting that eutrophication (due to excess of nutrient loadings, mainly N and P) affect primary production and subsequent chlorophyll-a and Kd (e.g. (Nixon 1995; Cloern 2001; Ryther and Dunstan 1971; Smith et al., 2006; Smith 2003; Carpenter et al., 1998; Herbert 1999; Duarte 2009; Duarte 1995; Nielsen et al., 2002b; Kemp et al., 2005).

We chose to focus on N input from Danish catchments (including both diffuse and point sources) in the scenarios, keeping atmospheric N deposition and Baltic sea waters nutrient concentrations unchanged (or implementing Gothenburg Protocol and BSAP for the mechanistic models). However, it is possible that part of the estimated reduction (in riverine N input) potentially could be "replaced" by a reduction in e.g. atmospheric N deposition.

Q: What data and evidence (published) exists that indicate which nutrient is limiting (N or P)? This may vary with season and location (e.g. Baltic/North Sea). How does this address diverse water bodies?

A: Published data on nutrient limitation in different Danish water bodies include analysis of DIN/DIP ratios (e.g. (Hansen 2016), ecological modelling (e.g. (Timmermann et al., 2010) , statistical modelling (Carstensen et al., 2007; Carstensen and Henriksen 2009, Møhlenberg et al. 2007) and nutrient enrichment experiments (Pedersen and Borum 1996; Pedersen 1995). These different publications also assess nutrient limitations supporting that N is the main limiting nutrient during summer across a wide range of the Danish water bodies.

Q: Nitrogen loading may be manageable, but is phosphorus in view of sediment exchange and large past efforts?

A: It has not been part of our assignment to analyse possible technical measures to achieve the calculated requirements to reduction of nutrient loadings; nor have the associated costs for managing nutrients (both N and P) been part of our assignment. Internal loading (of both N and P) is of course influencing the actual environmental condition. The Danish water bodies are relatively well flushed, and according to model results a new steady state between riverine loadings and nutrient pools in the sediment will be established over time resulting in lower benthic nutrient fluxes as a result of reduced riverine loadings

Q: In most systems, there is a gradual decrease in N loading that is not synchronous with the historical decrease in P loading. Which factors or policies have caused this decrease, and what is the expected autonomous trend in N loading under existing policies? Is there any quantitative information on this?

A: Beginning in the 1960's and accelerating through 1970's and 1980's increased application of N fertilizers and effective removal of P from wastewater and ban of P in detergents in mid-1980's (in some countries earlier) lead to high N:P ratios in streams and coastal waters potentially resulting in P-limitation in some estuaries – especially during spring. So, yes, there are factors (implementation of measures, changes in agricultural practice, waste water treatment etc.) explaining the historical decline in Danish nutrient loading as well as influencing the expected autonomous trend and predictions of future loadings resulting from different potential nutrient management scenarios. Past and future development in nutrient loading is, however, not within our area of expertise but we can recommend the following literature (in Danish): (Thodsen et al., 2016).

In the present study we have assessed the reductions targets compared to the average 2007-2012 loadings. The implementation of the Danish RBMP 2015-2021 include estimations on the trend in N loadings under existing policies, and the reduction targets has been corrected accordingly by the authorities. This is, however, not a part of the present study.

Q: How important is the interaction between N and P reductions and does the exclusive focus on N jeopardize the chances of reaching good status by the methods proposed here?

A: The model scenarios have mainly focused on N reductions (as the indicators were mainly N sensitive) keeping other factors (including P loading) constant. According to the model results, Danish marine systems will approach (and most of them also reach) GES under current conditions (climate, P loading, fishery etc.) if N loadings from Danish catchment is reduced. However, e.g. increased P loadings or changes in other factors (climate, nutrient from other sources, fishery etc.) may potentially challenge the ability to reach GES. If the current situation changes significantly, recalculations have to be made.

It should also be noticed that the implementation of BSAP, as a minimum, is a prerequisite for the possibilities to reach GES in the more open parts of the Danish waters. Here we do not expect that reduction in Danish N loadings alone is sufficient to reach GES.

Q: Has N:P stoichiometry as a determining factor for phytoplankton composition been considered?

A: Phytoplankton composition can be important for assessing water quality, especially if blooms of toxic algae or cyanobacteria are occurring. However, despite the comprehensive data records on phytoplankton composition in Danish waters, it has not been possible to develop a meaningful operational WFD indicator for phytoplankton composition. Due to the lack of a suitable indicator, and since neither toxic algae nor N fixating cyanobacteria are important in the majority of the Danish marine waters (Jorgensen et al., 2014), we have not tried to link N:P stoichiometry and/or nutrient loading to phytoplankton composition but focused on chlorophyll-a as the only intercalibrated phytoplankton indicator.

Q: Very important for the societal discussion: is the exclusive focus on (diffuse) N loading leading to the economically and societally optimal solution for the water quality problems? Is there evidence that it leads to the best results in comparison with the costs of the measures? Have any analyses been made of the cost aspects of the efforts required?

A: This is an important question, but it has not been a part of the present project.

Q: Apart from N-runoff from land (chosen as the primary concern) there are other factors that may affect Ecological Status. P loading has been mentioned. Also fisheries, habitat modification, change in the species composition of benthos have been mentioned in the literature, especially as influences on seagrass distribution. Have these factors been considered somehow, and is there evidence they are unimportant compared to land-based N runoff?

A: As described above the addressed indicators are known to be sensitive towards eutrophication and the mechanisms are well established. Furthermore, in the present study N load turned out to be the main eutrophication factor controlling the applied indicators. Although the list of hypothetical pressures is very long, the ranking of pressures (with regard to their quantitative effects) is limited by the lack of evidence based and quantified link between the pressure and a certain indicator (not the least lack of spatially and temporally resolved data is a main obstacle to the required multi-pressure studies). E.g. one might speculate that fishery may affect chlorophyll-a concentration due to trophic cascade effects, but this is very hard to document and the link between chlorophyll-a and fishery have not been demonstrated in Danish

coastal waters. Model sensitivity tests have shown that changes in zooplankton influence chlorophyll-a concentrations in inner Danish waters (Petersen et al., 2017). However, to our knowledge changes in zooplankton biomass/composition have not been linked to fishery in Danish waters. Likewise, trend analysis have indicated a shift in benthic fauna from filter feeders towards deposit feeders in Danish waters perhaps as a response to decreased phytoplankton concentrations (Riemann et al., 2016), but it is unclear if, or to what extent, this might influence e.g. chlorophyll-a concentration. During the last decades, potential pressures hampering eelgrass re-establishment have been studied extensively revealing a suite of factors affecting eelgrass growth and distribution depending on the local environment (Flindt et al., 2016; Canal-Verges et al., 2016; Valdemarsen et al., 2010; Pedersen et al., 2004; Koch 2001). However, light availability is documented to be one of the main factors controlling eelgrass depth limit (Duarte 1991; Duarte et al., 2007; Ralph et al., 2007; Nielsen et al., 2002a), which has been adopted as the indicator by the Danish Authorities. It is very likely that extensive studies may document and quantify additional pressures (besides eutrophication) that, at least to some extend may affect long term changes in e.g. chlorophyll-a concentration or light climate, but it is not likely that other factors may be more important than eutrophication given the vast amount of evidence of the importance of excess nutrient supply for these indicators. Future climate changes will likely exacerbate effects of eutrophication and induce changes in marine ecosystem functioning and structure. However, we do not expect this to be of great importance towards year 2027, and have not analysed this in more details as part of this project.

The adopted strategy to derive regionalized reduction targets for nutrient loading

In principle, nutrient reduction scenarios in a country can vary from a general, country-wide reduction target, over regionalized targets to water system specific targets. This document leads in the end to the definition of regional targets, but that comes as a surprise to the reader. The statistical modelling chapters suggested that water body specific targets would be defined, while the mechanistic model, based on country-wide reduction scenarios, suggested that one would arrive at a single national target. In the end, a regionalisation based on a set of aggregation rules were derived.

In general, there are arguments in favour of one national target (e.g. setting a level playing field for agriculture, simplicity of control, simplicity of communication, incorporating mutual influences between systems through coastal waters) but also in favour of specific targets (e.g. not overdoing efforts, optimal economic strategy). In the document, however, these arguments have not been made explicit and have not been the subject of extensive discussion.

Questions and answers

Comment: The aim of the project was to develop water body specific reduction targets to ensure the fulfilment of GES for all Danish water bodies. Hence, we have tried to estimate these reduction targets as individual targets for as many individual water bodies, and corresponding catchments, as we find possible from a model perspective, both taking into account the specific estuary characteristics and exchange with surrounding waters. The WFD operate with typology (which could be interpret as some kind of regionalization) and the Danish authorities has also divided the Danish water bodies in different types, which we have adopted in a modified version, as described in the scientific documentation. We are presently discussing a project description with the Danish EPA on an update of the typology applied towards the RBMP 2021-2027.

Q: Procedural: When was it decided to adopt this regionalized strategy? Who decided this? Were the current scientific results used as a basis for this strategy? If so, how was this done precisely?

A: We believe this question reflects some kind of misunderstanding, which indicate that our description does not fully describe the final procedure. Both during the development of the statistical models and the mechanistic models, we aim at setting up specific models for specific water bodies in order to provide water body specific nutrient reduction targets. For the statistical models, this is obvious, as it is the site-specific monitoring data that forms the input data to the model development, whereas we use the surrogate model approach (section 8.4.5) to calculate similar water body specific cause and effect relations when applying the mechanistic model approach. The nationwide N-load reductions (15%, 30% and 60% reductions) applied to the mechanistic models is solely to develop site-specific responses to N-load reductions (i.e. the surrogate models). The site specific surrogate models also depend on reductions in the boundary water bodies. However, we assume that the surrogate models can be used individually for enclosed local models. For the open waters, we use a kind of regionalization since open water bodies are highly interrelated and connected. The regionalization of reduction targets in open waters builds on calculated water body specific reduction targets, which have then been averaged over several connected water bodies (regions) such as the area around Samsø and Århus (blue area in Figure 8.19). In this area, K_d reduction targets based on the individual water bodies are 15% for Ebeltoft Vig, 19% for Kalø Vig (inner part), 13% for Århus Bay and 35% for the area around Samsø. However, this area is well flushed and well connected and surface waters mixes greatly, why we do not find any reasoning for dividing the open (regional) waters in to specific water bodies. This was based on a DHI decision and was formed while developing the methods to move from mechanistic model scenario results to final reduction targets.

Hence, for all water bodies upstream the open waters shown in Figure 8.19 we aim at water body specific reduction targets. Hence, we do neither adopt to a country-wide reduction target or regionalized reduction targets. We have tried to develop water body specific reduction targets where ever possible, however, adopting some kind of regional reduction targets for open waters. This should also be evident from Figure 8.23. Here the different reductions are shown on a catchment scale.

Q: How sure can we be that the regions are sufficiently homogeneous in their water bodies? In particular, when a regional target is low because most water bodies are open with short freshwater residence time, the region may also contain some sensitive, more isolated water bodies that would suffer from the low targets. Is this the case? How was it controlled?

A: We believe that this question reflects the same misunderstanding as mentioned above. As mentioned above, we only apply the regional approach in open waters where freshwater residence time is short and presumable well flushed and well mixed with boundary water bodies. For enclosed and more isolated water bodies we apply water body specific reductions. The procedure for setting specific reduction targets is described in section 8.7.1.

Q: The scenarios used for the mechanistic modeling use boundary values that are (in part) determined by nation-wide reductions of nutrient loading with a certain percentage. If there are regions with mostly open water bodies and low reduction targets, the actual boundary conditions for all of these water bodies may differ from the modelled ones, since the reductions in the coastal area will be less. There is, thus, a discrepancy between the modeled policy and the actual policy. Will this affect the results of the study? Is it possible that the reduction strategy for these regions is too low, because it is the regional rather than the local reduction percentage that will influence the ecological status?

A: It is correct that some discrepancy between the modelled policy and the actual policy exists. The adaptation of surrogate models leads to different individual reductions targets, whereas the development of the surrogate models assumed uniform reductions. For the open waters, we see lower needs for reductions than for enclosed and isolated water bodies, where we generally find the largest needs for reductions, and the resulting effects have not been assessed due to time constraints. However, DHI and MST are presently working on a project that will look into this as well.

The modelling of the accumulated reduction targets may suggests local adjustment to the reduction requirements originating from the surrogate modelling approach, but it is not expected to reveal substantial underestimations in any waters. Considering e.g. the estimated requirements for open waters, obviously reductions in one region influences reductions in neighboring regions but generally, the largest open water reductions are found in most southern water bodies, like the Little Belt region (39%), Great Belt region (20%) and the Sound region (18%) (see Figure 8.19). As surface water primarily is northbound the larger reductions in the southern regions influences the more northern parts with lower reduction needs. Hence, when reducing more in the southern parts we do not expect that the reductions in the more northern parts of the open waters are insufficient.

Furthermore, applying the strategy in section 8.7.1, the estimated reduction targets in coastal areas or upstream estuaries, that are less restrict than the down-stream reduction targets, have been substituted by the down-stream reduction targets.

It is also correct that the results from the open waters constitute the boundaries for the local models – and as the target reductions in the open waters are generally lower than for the estuaries and isolated water bodies, the effects from boundary reductions are less pronounced. Consequently, there is a much closer

link to the local nutrient loads, assuming that the boundary condition is not of decisive importance. This is an assumption, and can be challenged, but as we generally do not see large changes in absolute, modelled values in the open waters we do not expect this assumption to change upstream reduction targets significantly.

The generally larger reduction targets in estuaries and isolated water bodies does on the other hand impact downstream water bodies and locally open water bodies will be imposed by larger reductions than the overall targets set for that specific region.

Q: The statistical modeling only focuses on within-system temporal trends and the causality in these trends. As far as we understand, no cross-system analysis, relating the hydrographical characteristics of the systems to their vulnerability to nutrient loading has been performed. Why hasn't this been done? It could have formed a scientific basis for the regionalisation, as well as a basis for investigating the sensitivity of the approach to within-region differences in water body characteristics?

A: We agree that it will be beneficial to expand the analysis of the systems across the different types based on both hydrographical and hydrodynamic characteristics. This will increase the understanding of the systems and reduce the uncertainties of estimates of MAI outside the monitored estuaries. That said, the meta - analysis is a cross system analysis primarily based on hydrodynamic characteristics. However, it is very likely that a future revision of the adopted typology as well a cross-system analysis would improve our understanding of system sensitivity and functioning.

Choice of indicators and their sensitivity to nutrient loading

Compared to the requirements of the WFD, only a limited set of indicators have been used. Only two of them (chlorophyll a and Kd) have been used across the two modelling approaches. This leaves a number of unstudied indicator variables with respect to the good ecological status:

- **Chl-a only gives an indication of phytoplankton biomass, not of composition. Thus it may miss occurrence of toxic blooms**
- **Kd is probably insufficient as an indicator of habitat quality for eelgrass. In particular, herbicide concentrations may be missed as an alternative explanatory variable. The literature on eelgrass in Denmark frequently mentions hysteresis and the occurrence of alternative stable states. It may be the case that low nutrient loading and high water transparency are necessary but insufficient conditions for eelgrass restoration - it would be very useful to bring forward quantitative arguments proving this point. However, it would still be needed to know what other factors contribute and how.**
- **The benthic index seems to be unresponsive and should be examined more closely or replaced**
- **Nutrient stoichiometry (N:P in particular) is not considered**
- **Toxic substances, in particular herbicides, might be needed as supporting physico-chemical variables**

Comment: As agreed with the authorities, the development of models and methods has been focused on two (out of three) indicators adopted by the Danish authorities: Chlorophyll-a and eelgrass depth limit. The depth limit has been transformed into K_d as described in the scientific documentation prepared for the international evaluation.

As the expert panel states, eelgrass development is dependent on a number of other conditions than light availability. Especially, the abundance and coverage are shown to be controlled by other factors than light availability (Koch 2001). However, the official indicator defined by the Danish authorities is the eelgrass depth limit and it has often been demonstrated that light penetration/water clarity is the most important factor controlling the depth limit (Duarte 1991; Dennison 1987; Nielsen et al., 2002a; Ralph et al., 2007). Therefore, it has been evaluated that Kd is a reliable proxy for the Danish bottom flora indicator.

Other indicators – intercalibrated or not – could be included towards the development of RBMP 2021-2027, and DHI and AU are presently having a dialogue with the authorities about including additional indicators.

Questions and answers

Q: Why are additional variables (e.g. days with nutrient limitation) used in the statistical modeling but not in the mechanistic modeling, especially as it appears that these variables correlate closely with chl-a and do not give much independent information?

A: The statistical models link external drivers (e.g. nutrients) to a single variable (e.g. chl a) but do not explicit include indirect effects of nutrient loading (e.g. primary production and oxygen depletion) which also affect chl a concentration. These interactions are more explicit included in the mechanistic models. In order to capture more of the complexity of the ecological functioning and provide a more holistic picture of ecological status several additional indicators were included in the statistical approach. The indicator “days with nutrient limitation” is an indicator for the degree of bottom up control of the system and a proxy for pelagic primary production. Although there is a link between primary production and e.g. chl a, primary production (or days with nutrient limitation) provide information of ecosystem functioning that is not captured by the chl a indicator although the indicators are often correlated.

Q: Could additional reference value targets be developed for TN and TP, using the same methodology as for chl-a? Presumably, these would be more directly related to loads and simpler to understand than the supplementary indicators used at present.

A: It is obvious to continue applying the developed models and set targets for e.g. TN and TP. We are sure this is doable, and we are presently having a dialogue with the authorities focusing on targets for TN and TP and potentially winter concentrations of DIN and DIP. How this will be effectuated and potentially implemented towards RBMP 2021-2027 is not entirely clear yet, but we are presently working on describing different methodologies.

Q: None of the models has been able to show a strong influence of nutrient loading on Kd, except when going from hypertrophic to eutrophic conditions. Why is Kd nevertheless given more weight (at least with the statistical modeling) than other variables?

A: In the statistical model approach, Kd has been given same weight as the chlorophyll-a indicator and double weight relative to the additional indicators used in the statistical approach. The Kd and Chl a indicators have been given double weight in order to reflect the importance of these indicators in the official ecological classification where only intercalibrated indicators are used. In addition, they are both of fundamental importance for ecological systems. In the calculation of total nutrient reduction requirement, the Kd indicator has a weight of 2/7.

In the mechanistic model approach the two indicators chlorophyll-a and Kd have similarly been given equal weight.

Q: What justifies the apparently arbitrary translation of calculated needed reductions (of N load in order to obtain target Kd) in the order of 200% to 25 %? Why 25 and not any other arbitrary number? Is the fact that unrealistic needed reductions are obtained, not a reason to decrease confidence in the models and downweight the importance of the variable in the final conclusions?

A: We fully acknowledge that the estimated slopes for nitrogen reductions versus Kd are low, leading to sometimes very high estimates for load reductions. However, for some areas, the slopes are higher and overall there is plenty of evidence that reduction in nitrogen loadings leads to a decrease in Kd (e.g. Lyngsgaard et al. 2014, Riemann et al. 2016). We also believe that we have a good hypothesis (accumulation of organic matter both in the form of DOM and particles leading to a considerable time lag) for the low slope values as explained in the report (section 8.3).

We do not find that our intervals for categorization of Kd-slope reductions are arbitrary at all, as suggested by the panel. The values for the categories (25-50, 50-75, and 75) are chosen given that fact that inter annual variation in N-loadings are in the order of 25% and the hypothesis that a change larger than then inter annual variation is needed in order to change the status of the ecosystems. We admit that values in the range of 20-30 % could also have been used, but we believe that values outside this range are unreasonable. This is an example were expert judgement is part of the overall analysis; something there is recommend in the WFD. In fact it illustrate our strategy for this project – to use objective statistical methods on observed data as far as it can be done and then supplement with expect judgement.

The suggestion of decreasing the weight or remove Kd as an indicator from the analysis was not an option. In the former WFD plan period, the depth limit of eelgrass was the only indicator used, based on an assumption with Kd and N-loadings. This was heavily criticized by the agricultural organizations. In this analysis, we have a much more diverse approach for evaluating the status of marine systems. However, as explained in the report (section 8.3) there are pro and cons for all indicators, and one of the strengths of Kd

indicator is the coupling to depth limits of eelgrass, which is the only indicator for which we have trustworthy observations for the reference conditions. In contrast, for chlorophyll-a concentration the reference conditions are based on estimates on loadings at the year 1900 and model estimates that necessarily are extrapolation far beyond the validation range.

Q: What is the impact of the (doubtful) Kd calculations on the final results? Would the results have been essentially similar without these calculations or is the dependency (and thus the uncertainty) on Kd results large? This is important to estimate the robustness of the results!

A: The governing assumption behind the estimated reduction targets is; when a water body (based on observations) does not fulfil the indicator targets, some actions are required. The modelling – supported by literature – suggest that the Danish indicators reacts to N loadings, why we estimate a reduction target when at least one of the two indicators does not fulfil the targets.

Based on the official water body classification, the chlorophyll-a target alone is not met in 18 water bodies, the depth limited (transferred into K_d) target alone is not met in 27 water bodies, and for 45 water bodies neither of the two targets are met[1]. Consequently, reduction targets for 27 out of the 119 water bodies are solely defined by the Kd target (averaged with a zero-target for chlorophyll-a).

As described in the scientific documentation prepared to the expert panel we carried out a sensitivity test. This test revealed that the reduction targets were most sensitive to the status and the targets, and less sensitive to the slopes. Varying the slopes by ±10% lead to changes in N-load reductions of ±2-3% on average, whereas changes in status and target values of ±10% lead to changes in load reductions of ± 10-11% on average. The Kd targets were based on historical observations of eelgrass depth limit and have not been assessed further in this report. Hence, we do not consider the overall reductions largely dependent on Kd, and the sensitivity does not indicate otherwise.

Q: Can you derive supporting evidence from the literature that shows that nutrient loadings affect eelgrass independent of Kd, or that nutrients and Kd are necessary but insufficient conditions for eelgrass restoration?

A: Light availability is a necessary but not sufficient factor for eelgrass growth and distribution. Whereas the maximum depth limit is often explained by light (Duarte 1991; Dennison 1987; Nielsen et al., 2002; Ralph et al., 2007; Duarte et al., 2007) several other pressures not necessarily linked to light (Kd) and nutrients including physical stress, frequent resuspension, epiphytes, sediment composition , hypoxia/anoxia etc. may affect eelgrass growth and restoration (Koch 2001; Canal-Verges et al., 2016; Flindt et al., 2016; Pedersen et al., 2004). The combination of realised pressures depends on the local conditions and even at sites optimal for eelgrass growth, recolonization may take years.

Q: Have you considered other measures than nutrient load reduction in order to restore eelgrass beds?

A: Eelgrass restauration is difficult, and research is ongoing (e.g. in the Danish research project NOVAGRASS, http://www.novagrass.dk/en). In this project we have not assessed measures for restauration, but assessed reduction targets to obtain sufficient light to support the depth limit indicator.

Over the past 3-5 decades anthropogenic activities have been affecting seagrass ecosystems globally leading to major loss of valuable habitats (Schmidt et al. 2012). In temperate seas, eelgrass historically

[1] For 17 water bodies no observations were available, and potential reduction targets are set according to downstream reduction targets

covered large areas in protected bays and estuaries, but because of eutrophication affecting light availability and epiphyte growth the extent of present eelgrass beds are only a fraction of healthy beds experienced around 1900 and in the 1960-ies (Krause-Jensen & Rasmussen 2009). In Denmark nutrient reduction load targets (80% for phosphorus and 50% for nitrogen) adopted in 1988 were met about 15 years ago but recovery of eelgrass beds is yet to be seen (Carstensen et al. 2013). Other pressures such as increasing summer temperature, changed sediment texture and organic content, or impacts from toxic chemicals such as herbicides have been suggested as potential pressures preventing eelgrass recovery (Koch 2001, Kaldy 2014, Krause-Jensen et al. 2011, Roca et al. 2016, Pulido & Borum 2010, Devault & Pascaline 2013).

The expert panel specifically requested information about potential impacts of pesticides (herbicides) on eelgrass health. Present use of herbicides (including desiccation products) in Denmark amounts to ca. 2.000 tons active substance per year (Miljøstyrelsen 2017). Most herbicides (and their degradation products) are rather water soluble and there is a risk that excess herbicides are transported to ground water or to streams draining agricultural fields. Herbicides are routinely monitored in Danish streams with Glyphosate (including the degradation product AMPA) and 2-6-dichlorbenzamid (BAM), being the degradation product of the banned 2,6-Dichlorobenzonitrile (Dichlorobenil) with highest occurrences and concentrations (Table 1). Compared to average and "extreme" (90-percentile) herbicide concentrations measured in freshwater streams (Table 1) we must expect even lower concentrations in coastal waters because of dilution. With that in mind and combined with estimated no-effect concentration (PNEC) at 398 µg/l (Maycock et al. 2010) impact of Glyphosate/AMPA on seagrass in Danish estuaries and coastal waters is highly unlikely. Besides AMPA, 2-6-dichlorbenzamid (BAM) occurs regularly in streams but in low concentrations 0.012-0.12 µg/l (Table 1). Although no EQS or PNEC values have been estimated for BAM, the 90-percentile freshwater concentrations are 4-to-6 orders of magnitudes lower than the concentrations known to cause toxic effects in aquatic organisms, including primary producers (Björklund et al. 2011). Hence, impacts on eelgrass population are unlikely.

Some abandoned herbicides such as TCAA are still present in the aquatic environment in measurable concentrations while others such as Atrazine must be regarded as a past phenomenon in Danish streams (Table 1). Compared to impact concentrations of in TCAA the mg/l-range the 90-percentile is 10-100.00 times lower in Danish streams. Therefore, TCAA-induced impact on eelgrass in Danish estuaries is not likely.

Two Danish studies addressing potential impacts of herbicides on eelgrass are worth to mention;

- Dahllöf et al. (2008) using passive samplers found 20 different herbicides in Nissum Fjord during the autumn 2007. The most freshwater-influenced (2-5 ppt) part of Nissum Fjord had the highest herbicide "concentrations". Applying freshwater "uptake rates" to the samplers concentrations of two "old" herbicides diuron and isoproturon (not sold for 6-7 years) were estimated between 0.14 and 1.76 µg/l (diuron) and 0.02 and 0.13 µg/l (isoproturon). Especially diuron is toxic to seagrass with increased mortality at 7.2 µg/l and sublethal effects at 1.7 µg/l measured after 79 days exposure (Negri et al. (2015). Compared to other estuaries the inner part of Nissum Fjord is not a typical eelgrass habitat because of low and fluctuating salinities. Low salinity imply low level of dilution of freshwater with seawater.
- Nielsen & Dahllöf (2007) compared impact on eelgrass "growth" (leaf-elongation) after short term (3 d) exposures to herbicides (Glyphosate, Bentazone, MCPA), applied as single toxicants or in mixtures. Single toxicant applications did not differ from controls even at the highest concentrations (Glyphosate: 170 µg/l; Bentazon: 240 µg/l; MCPA: 200 µg/l), while "growth" was about halved compared to controls when herbicides were applied in mixtures at "low"

concentration (A: 170 µg Glyphosate/l + 2.4 µg Bentazon/l + 2 µg MCPA/l) thereby indicating synergistic effects. Compared to recent concentration levels measured in streams (Table 1) the experimental concentrations are highly unrealistic and it is questionable if such observations can be used to predict impact of herbicides in Danish estuaries and coastal waters.

To conclude, apart for nutrient loads most probable sediment quality (including H_2S) and high temperatures stimulating respiration are those factors preventing fast recovery of eelgrass.

Table 1. Overview of results from Danish monitoring for herbicides in streams

Pesticide	Type of monitoring	Period	Stations/sampling	Finds	Avr. Conc	90% percentile
				%	---- µg/l ----	
2,4-D	Control	(2006)	1/12	17	<DL	<DL
2,6-DCPP	Control	(2006)	1/12	0	<DL	<DL
2,6-Dichlorbenzamid	Control	(2006-2013)	16/185	63	0.016	0.029
(BAM)	Operationel	2012	12/125	51	0.012	0.029
	Other	(2004-2011)	13/24	92	0.041	0.12
4-CPP	Control	(2006)	1/12	0	<DL	<DL
4-Nitrophenol	Control	(2006-2013)	16/185	23	0.012	0.044
	Operationel	(2012)	12/125	8.8	0.012	<DL
	Other	(2004-2011)	1/12	26	0.014	0.029
AMPA	Control	(2006-2013)	16/185	80	0.12	0.28
	Operationel	(2012)	12/125	87	0.16	0.27
	Other	(2004-2011)	8/19	95	0.11	0.22
Atrazin	Control	(2006-2013)	16/185	1.1	<DL	<DL
	Operationel	(2012)	12/125	0	<DL	<DL
	Other	(2004-2011)	8/19	0.01	<DL	<DL
Desethylatrazin	Control	(2006)	1/12	0	<DL	<DL
Desisopropylatrazin	Control	(2006-2013)	16/185	1.1	<DL	<DL
	Operationel	(2012)	12/125	2.4	<DL	<DL
	Other	(2004-2011)	1/12	0	<DL	<DL
Hydroxyatrazin	Control	(2006-2013)	16/185	2.7	<DL	<DL
	Operationel	(2012)	12/125	13	<DL	0.011
	Other	(2004-2011)	10/23	0	<DL	<DL
Bentazon	Control	(2006-2013)	15/173	13	<DL	0.021
	Operationel	(2012)	12/125	17	<DL	0.025
	Other	(2011)	1/12	17	<DL	<DL
DEIA	Control	(2006-2013)	16/185	2.2	<DL	<DL
	Operationel	(2012)	12/125	12	<DL	0.011
	Other	(2004-2011)	8/12	5.3	<DL	0.022
Dichlobenil	Other	(2004)	5/5	0	<DL	<DL
Dichlorprop	Control	(2006)	1/12	0	<DL	<DL
Dinoseb	Control	(2006)	1/12	0	<DL	<DL
Terbuthylazin	Control	(2006-2013)	16/185	4.3	<DL	<DL
	Operationel	(2012)	12/125	4.8	<DL	<DL
	Other	(2004-2011)	8/19	0	<DL	<DL
Terbuthylazin (hydroxy)	Control	(2006)	1/12	8.3	<DL	<DL
Trichloro acetic acid	Control	(2006-2013)	16/185	50	0.047	0.11
(TCAA)	Operationel	(2012)	12/125	30	0.079	0.073
	Other	(2004-2011)	8/19	16	0.057	0.42

Basic strategy of the statistical modeling

The statistical modelling focuses on within-system short-term models, resolving both long-term trends, seasonal variation and year-to-year variation that correlates with freshwater discharge. This is a choice, but alternatives could have been chosen.

Comment: It is not correct that our method is resolving seasonal variation. On the contrary, we are deliberately avoiding this because we think that would be unsound for two reasons. First, only in very small estuaries with a large inflow, we can expect significant effects of short time (days, weeks or up to a few month) events in freshwater and hence nutrient inputs. Almost all Danish estuaries are likely to integrate the pressure over a longer period. Secondly, in the evaluation of status in a WFD context, the criteria are annual or several years values of an indicator.

One could have concentrated on long-term trends only, e.g. by correcting yearly values for freshwater discharge as is often done in Danish literature.

Comment: For small estuaries like the Danish, most (about 90%, see e.g. Thodsen et al. 2016) of the interannual variation on a five-year scale, in nutrient input comes from inter annual changes in freshwater discharge. Thus, by normalizing an indicator to freshwater input, most of the variability in nutrient loadings is removed. It is very unlikely that freshwater in itself has an effect on eutrophication. Only over a longer time scale, changes in freshwater-specific loadings become important. Ideally, e.g. with a 100-year time series, normalization to freshwater discharge could probably work, but we are far from having that long time series. The often used practice to normalize a marine variable to freshwater runoff is a short cut to take into account the effect of nitrogen loadings (before mid-1990s) or the combined effect of nitrogen and phosphorous loadings (after mid-1990s where most of both N and P come from the open land). The fact that this practice often works, further support the dominating effect of nutrient loadings for the ecology of Danish estuaries.

One could also have chosen to model the cross-system differences as a function of hydrographic conditions (e.g. fraction freshwater in some form, stratification,…), thus enabling an evidence-based typology of systems, rather than the current (and unclear) basis for the typology. It would also have given an evidence base underlying the meta-modeling. At first sight, a long-term and cross-system approach would have fitted the purposes of the study better.

Comment: The typology was a given precondition as it is the official typology reported to the EU under the WFD. We agree that the assessment work could most likely benefit from a revision of the typology/a more cross-system-based approach as we also state in the report. MST, AU and DHI have initiated a project with the aim to evaluate and revise the typology, which could support the MAI estimations especially for meta water bodies and estimation of chlorophyll a reference values. Relevant criteria could be catchment/volume ration, mean depth etc. However, the lack of relevant data especially for the “meta water bodies” as well as sufficient cause-effect relations will most likely constrain the approach.

A second basic choice has been to detrend all independent variables, except the nutrient loadings, and not to detrend the response variables. This necessarily inflates the correlation between nutrient loadings and response variable, in case the latter shows trend: the trend can only be attributed to the nutrient loadings, also when in fact it would have been caused by climate change, increased freshwater extraction or other causes.

A third basic choice has been to select independent variables on MLS, and then apply regression models using PLS. This combines the sensitivity of MLS to colinearity in independent variables, and the bias in

slope estimators (when applied for prediction) of PLS. The most important consequence of this choice is that only one nutrient loading can be selected, and combined effects of N and P loading, or their interaction, cannot be resolved by the models. Another consequence is that in some systems neither nutrient is selected as affecting the response variable, thus leading to a logical problem in estimating needed levels of reduction. Given the large knowledge on aquatic ecological processes, one wonders why variable selection has been needed in the first place, and why the modeling was not based on more advanced models that could have taken into account colinearity.

A final basic choice has been not to perform an explicit sensitivity analysis, or to report on the uncertainty of the results. Several methods to do this properly exist, both for within-system studies (e.g. based on Bayesian approach) and especially for between-system studies in a metamodeling or typology-based grouping of systems. Lack of communication about uncertainty of the findings hampers communication with stakeholders and induces risks of economic or ecological damage (in cases of overdoing, resp. underdoing).

Questions and answers

Q: Why has the choice been made for short-term, within-system models? Why are these better than alternatives?

A: The basic argument for 'within-system' models is that this is required in the WFD. In our interpretation, which is supported by legal experts (see e.g. Anker 2016 and citations in Altinget 26-02-2016), the obligation for the member states is to ensure GES for each individual water body. In principle, this requires an analysis of the status and the pressures on each water body, and then an estimation of the combined reduction of one or several of the pressures in order to bring the individual water bodies in GES.

Denmark has reported 119 marine water bodies in the WFD. In principle, the above-mentioned analysis should therefore have been made 119 times. This is a very ambitious task, which is hampered by the fact that we do not have monitoring data for the majority of the water bodies. As mentioned in our report, long-term data (more than 15 years with annual sampling) are available for 29 stations covering 23 water bodies. For the remaining about 81% of the water bodies, there is either no or only sporadic monitoring data. As far as we understand, this situation with limited data coverage is similar to the situation in most member states.

The lack of sufficient monitoring data for several water bodies poses a challenge and we have used a typology approach to extrapolate model results to adjacent water bodies with similar typology. The WFD is typology based (e.g. for establishing reference values) and as such there is consistency between WFD indicator target setting and e.g. the meta-model approach. However, a revised typology/cross-system analysis could potentially improve the cause-effect relations provided that we have sufficient monitoring data to derive the models and meta-data. As aforementioned the long term analyses are constrained by the length of the data series and as stated in the report (p 46-47) we consider the next logical step in the statistical modelling approach to be a Bayesian hierarchical modelling of cross-system data as seen in e.g. (Borsuk et al., 2004).

Two secondary arguments for a 'within-system approach':

From a scientific point of view, the Danish water bodies are highly diverse spanning large gradients in depth, salinity, and impact from the catchments and from other press factors, e.g. mussel dredging. Thus, it is necessary to treat each water body individually. That said, there are similarities, which is why we have

grouped the water bodies into e.g. the estuaries on the east coast of Jutland (see also below about typologies).

The last argument for the 'within-system approach' is the combination of historical reasons and time constraints. The technique was first undertaken in the late 1990s, specifically for Mariager Fjord, after an event in 1997 where the estuary went completely anoxic emitting free H_2S to the atmosphere. The technique was further developed and applied during the 00s but only for individual estuaries. When the Danish government initiated the project in 2013, with a time frame of 1.5 years and a limited budget, we had to rely on existing data and techniques.

Q: What justifies the choice for models that exclude the probing of interaction between different nutrients, one of the major problems in the current study?

A: The technique as such does not exclude probing the interactions between the nutrients nitrogen and phosphorus. In fact, the technique has successfully been used for that purpose in an earlier study about the estuary Limfjorden published in 2006 in the report Markager et al. (2006). However, this report used data from 1985 to 2003, where there was a clear decoupling of changes in loading of phosphorous and nitrogen in the data. The successful reduction in phosphorous loadings from sewage treatments plants (about 90 %) means that today – and in the data from 1990 to 2012 used for this analysis - both phosphorous and nitrogen are predominantly coming from the diffuse sources and therefore co-vary with each other and with freshwater run-off (see also section about N and P). Separating co-varying variables is always a challenge in statistical modelling and in order to overcome this and qualify the parameter selection in water bodies where N and P loadings are co-varying, we have performed an analysis of nutrient limitation .

Q: What justifies the variable selection procedure, given that the emphasis was not on proving the effects of nutrients on water quality, but the estimation of the regression coefficients?

A: We are somewhat puzzled about this question. In our view, any regression technique involves a selection of explanatory variables, one or in the case of MLR several variables. The strength of MLR is that it allow probing interactions between explanatory variables, and that is what we believe we have achieved for nutrient loading versus the other variable. However, even with the PLS-technique a high degree of co-variation poses a problem. Thus, simultaneous estimation of coefficients for N and P loadings can be problematic. In the report (page 35), we have described how we have used accepted and well-described statistical techniques and also that we have compared 'free' and unconstrained solutions with solutions with N and P as preselected explanatory variables. See also section about N versus P in general. As stated there, we disagree with the view that differentiating the effects of N and P 'is one the major problems'.

Q: How reliable are the estimates of influence of nutrient loadings, given the strategy of detrending applied?

A: It is clear that the detrending of other variables than N and P will relate trends to put more weight on the effects of changes in N and P versus indicators that show a trend. However, a choice of not detrending would mean that a trend in a climate variable, in this case wind, will get a substantial effect and take part of the effect away from decreasing N-loading and put it on the observed decrease in wind (This was realised during the development of the models). Given our knowledge about marine systems, we find it less likely that wind will have a large effect on e.g. TN concentrations. However, it is not impossible to come up with a mechanistic hypothesis where wind does affect TN concentrations; but it is likely less likely than the hypothesis that N-loadings are the main driver of the observed TN-concentrations.

Q: Why have no measures of uncertainty been formally derived and presented in a way that is easy to understand for stakeholders? This could make the recommendations clearer and more acceptable. (e.g.https://www.ipcc.ch/pdf/supporting-material/uncertainty-guidance-note.pdf)

A: We have used several traditional statistical measures (R^2, RMSEP etc.) in order to assess model uncertainty/model reliability. These measures are focused on the ability of the model to predict individual indicators (Chl a, Kd etc.) which is important, but these measures are not assessing the uncertainty related to predictions of MAI. Dealing with uncertainties related to complex calculations such as MAI, which involves status values and reference/target values for several indicators, expert judgements as well as models and extrapolations etc. are far from trivial and there is no formal way to estimate the uncertainty. In addition, it is not possible to compare model predicted MAI-values with observations which further hamper a traditional uncertainty analysis. Instead, we have applied sensitivity tests and ensemble modelling where possible. This approach is also used in e.g. climate predictions and weather forecasts where traditional uncertainty analysis is difficult/impossible. The rationale behind the ensample modelling is that if predictions of MAI using two independent model approaches are almost similar and significantly correlated, then it is unlikely that the uncertainty of the individual models is large (assuming no model bias in both model approaches). In addition to the more quantitative assessments of model uncertainty that we have performed (using statistical measures, ensample modelling and sensitivity tests), we have indeed tried to convey the uncertainties in the text and on many meetings during the process.

We totally agree with the panel about the importance and the desirable in trying to convey uncertainties to managers and stakeholders. However, we also find this the most difficult part to communicate. The panel refers to the IPCC material. However, reading it reveal a statement like:

'Be prepared to make expert judgments in developing key findings, and to explain those judgments by providing a traceable account:'

We actually find that this is precisely what we tried to do in both our original report in Danish, in popular articles, in countless interviews in TV, radio and new papers and on meetings, but communicating uncertainties (whether they are quantified or more qualitative) is challenging.

Basic set-up and validation of the mechanistic models

In general, the model set-up is clear, but details of the processes and parameters are not easy to find, especially as some of the referred documents in the model description are not publicly available. In the general set-up, it is not entirely clear why in the end four different models were set up, especially as the use of a flexible mesh would have allowed to use a single model with spatially differing resolution. You mention in the description that the IDW model differs from the estuarine models in some process formulations and variable settings, and you give arguments why that has been done. We assume that you split the estuarine models in different models for practical reasons, but would like to know why. More importantly, we do not know if these models were the same in variables and parameters, and thus only differ from one another in bathymetry and boundary conditions. If settings differed, we would need details on the how and why.

Model validation was presented based on average values per month and water type. However, in the present setting a crucial validation element for the models is whether the models have been able to capture the long-term trends in water quality as related to reductions in nutrients. Evidence showing the model behavior in this respect should be easily obtainable from model output.

Questions and answers

Q: **Can you provide us with a copy of the documents you refer to in the model description?**

A: We assume it is the DHI documents you are referring to. Hence, these have been attached. If you also were referring to other documents detailing the model description, please get back to us. For practical reasons we have included the 2016 version of the references, but differences between the latest and earlier version are insignificant.

Q: **Can you give more details on the four models, and what are their differences and similarities?**

A: Basically, we have adopted two different biogeochemical models (i.e. two different sets of state variables and processes); one for the IDW model and one for the estuarine models. In the DHI references forwarded to the panel as part of the answers to this group of questions, the state variables and processes are described for the IDW biogeochemical model (DHI 2016). The differences between the two models are highlighted in Table 7.1. This table highlights the functional differences between the two different biogeochemical models. The functionalities not highlighted are more or less identical formulations in the two models.

Setting up four different models in the end instead of having one model including both estuaries and the IDW model is based on combinations of different arguments:

1. A practical argument is that the CPU demands would raise, and time for each model run would increase significantly. The models are based on flexible mesh and in the IDW model the resolution varies between approx. 300 m to >6 km, whereas the estuarine models have grid cells less than 100 m for the finer grids, and down to less than 30 m in e.g. Odense Fjord. We did try to increase resolution in the IDW model to less than 300 m locally, but the increase in CPU time did not allow for this approach.
2. A process and data argument is that the estuarine models includes a tighter coupling between the benthic and the pelagic compartments and also include inorganic sediments subject to resuspension, and adsorption/desorption of PO_4 to inorganic sediments. These processes can be equally important in the IDW model, but the demand for sediment data for this benthic-pelagic interaction calls for more data than what is available in the open waters. Hence, especially the

sediment interactions are described in less details in the IDW model compared to the estuarine models.

In the three estuarine models, identical biogeochemical model formulations are used. Due to local differences (system and data), the set of calibration constants are not entirely identical for all three setups. However, the model consists of approx. 275 different constants, and less than 10 of those constants differs between the estuarine setups. All the constants that differ are associated with the sediment.

Q: **Can you specify details on the atmospheric forcing: Was only a single year used, whereas Denmark reports on atmospheric deposition to Helcom for longer periods? How was the atmospheric N deposition divided over different species? Was atmospheric P deposition considered?**

A: With respect to atmospheric depositions, we apply modelled N depositions for each single year of the period 2002-2011 (i.e. monthly averages for 2002 to perform biogeochemical modelling of year 2002, etc.).

The atmospheric model is developed by AU and they were responsible for delivery of the required data. The model was first applied in 2007 and have been used since then for estimation of national atmospheric inventories, e.g. to HELCOM. All years have been executed based on specific emissions and meteorology of the specific year. For the ecological modelling, we only considered the inorganic nitrogen fractions (NH_4^+ and NOx) of the wet and dry deposition, which is delivered as output of the atmospheric modelling. The dry and wet depositions of each species are lumped and applied as input to the surface concentrations of NH_4^+ and NOx in the model.

Q: **In shallow waters assumptions with respect to atmospheric deposition input can be crucial and potentially allow a manipulation of the MAI. Was the deposition data spatially resolved? If not, how was it taken into account in the model? Were gradients between land and sea taken into account? Which atmospheric N fractions were considered as bio-available in the model and how were they calculated? Was the atmospheric input of P fractions considered, as well?**

A: The atmospheric model was executed with a grid resolution of 16 km in order to handle the land-sea gradients. In order to handle gradients in the deposition velocities at the different surface types the model have different deposition velocities for the different surface types (different forest types, different crops, grass etc, and open water). It is only the total deposition to open waters (with a spatial resolution of 16km), which have been used as input to the mechanistic biogeochemical model.

The yearly reports (in Danish) also include some indication on resolution and spatial distribution of the N depositions, see http://www.dmu.dk/pub/fr708.pdf, http://www.dmu.dk/pub/fr761.pdf, http://www2.dmu.dk/pub/fr801.pdf, http://www2.dmu.dk/Pub/SR2.pdf and http://www2.dmu.dk/pub/sr30.pdf for the specific years: 2007 to 2011.

Q: **Can you provide us with the validation data showing that the models have been able to capture the essential effects of nutrient reduction on target variables chl-a and Kd?**

A: We have run the models for a period of 10 years: 2002-2011. During that period no significant trend in loads are observed, why we cannot, through verification data, show that the model is able to capture the essential effects of nutrient reduction. However, as we find similar cause-effects (slopes) compared to the statistical models, we conclude that the models respond to the loadings, as has been observed historically. To be able to evaluate the models comparing to the historical load reductions we should have modelled at least 10 more years.

Q: **No estimates of model uncertainty were given. Do you have any estimate, what is it based on and what is the order of magnitude of the estimated error on the variables of interest (in particular the derived nutrient reduction need)?**

A: As for the statistical models, we have used traditional statistical measures in order to assess model uncertainty/model reliability for the mechanistic models. These measures are focused on the ability of the model to predict individual indicators (chlorophyll-aa, Kd etc.) which is important, but these measures are not assessing the uncertainty related to predictions of MAI. Dealing with uncertainty of predictions in complex ecosystem models is far from trivial, because of potential errors and uncertainty associated with input data, the initial conditions, data used for calibration and model structure. With 10 years input data including > 300 nutrient sources in Denmark alone, more than 275 model constants and 60 state variables it will be impossible, due to computationally capacity, to apply proper uncertainty analysis (Monte-Carlo) similar to what is often done for simpler hydraulic river models.

As an alternative approach multi-model ensemble modelling to determine model prediction uncertainties may be used as in the climate change community (Weigel et al. 2008). Application of a "truth" ensemble approach will require multiple models covering the same area, time period, each using the same set of input data and preferentially also use comparable model resolution (Pogson & Smith 2015). Previously, post-hoc ensemble modelling (4 different models) have been used to assess "problem areas" due to eutrophication in the North Sea and the Baltic Sea (Almroth & Skogen 2010).

True ensemble modelling has not been possible in this project, however, as described in the scientific documentation we did introduce some reduced ensemble approach. Having very different and independent model approaches covering overlapping water bodies did result in quite similar reduction targets. Hence, it is unlikely that the individual model uncertainties are large.

In addition, we have compared the slopes between nitrogen load and response variables (summer chlorophyll-and Kd) estimated with the mechanistic models and the statistical models. During the 10 years of modelling carried out as part of this project, we do not see any significant trends in measured concentrations of either N, P or chlorophyll-a. This is also expected as the loads from Denmark (Figure 2.2 in the scientific documentation) and from neighboring countries (HELCOM 2011) during that period is fairly uniform. However, as the response in the mechanistic models (based on N load reduction scenarios) show similar slopes as compared to the statistical models using historical load reductions going back to the period before significant nutrient load reduction are introduced, we find it most likely that the dose-response in the different water bodies is reflected in the mechanistic models.

At present both AU and DHI participate in a Danish research project (http://seastatus.dhigroup.com/) where one keyaim is to define methodologies for estimation of model uncertainties. If anyone in the expert panel has some advice on how to proceed with estimating model uncertainties, this will be highly appreciated.

Consistency between target values in statistical and mechanistic modeling

Both the statistical model chapters and the mechanistic model chapters describe how reference conditions and target values were defined. In the 'ensemble modeling', as well as in the meta-modeling, the targets from both model approaches are considered sufficiently consistent to be used in averaging procedures.

Questions and answers

Q: **Are these target and reference values conceptually consistent across the two modelling approaches? As far as we understand, the statistical modelling extrapolates back from the present situation in a particular water body to the situation that would be present if the *local* nutrient loading would be reduced to 1900 levels. This does not take into account the reduction in background marine values, nor the effect of local Danish reductions in other waters that reach the system of interest through the sea. It also does not take into account regional (e.g. BSAP) efforts. This reference value, therefore, must be significantly higher than the reference value calculated with the mechanistic model (which assumes both N and P reduction to 1900 levels, in both the system of interest and the whole world around). The reference value of the statistical model would be much closer to the '*target obtainable through Danish land-based N reduction*' in the mechanistic model. In terms of fig. 8.14: the intersection of the orange slope line with the upper dotted horizontal orange line, and not the point with the red cross. Can this relation between the definitions of the reference and target values be clarified, and can arguments be given why the approaches from both model strategies are nevertheless conceptually similar enough to be averaged?**

A: In contrast to the mechanic models, the statistical models do not take non-Danish N loadings into account and therefor these models are only applied in water bodies where N load from Danish catchments are assumed to be dominant. For these water bodies the intersection of the orange slope is approximately in line with the point marked by a red cross for the mechanistic models, indicating that non-Danish N load is of minor importance. For areas where local Danish N loads are dominating the two model approaches will be simulating the same reference-scenario (although the methods are different).

Meta-modelling

While in general the strategy for meta-modeling is clear, there is a question regarding the North Sea waters on the Jutland coast, and a request from the panel for more supporting data.

Questions and answers

***Q:* Can you explain how 'meta-modeled' results for North Sea waters could be derived, when none of the underlying models has considered this type of waters, which differ from all other water bodies in tidal range, temperature regime, sediment loading, nutrient concentration, stoichiometry and possibly a suite of other characteristics? Have the same indicators and criteria been used for North Sea and Baltic estuaries, and is this justified?**

A: For the North Sea area, only the chlorophyll indicator is involved in investigation of needs for nitrogen reduction as the environment along the North Sea coast does not support eelgrass meadows. As determined by the EU intercalibration procedure, this indicator evaluate the 90-percential chlorophyll-a concentration from Marts to September. In the present project we assume that the meta-model effect from N on chlorophyll-a are similar in the North Sea as within the Kattegat and Baltic Sea area, and we apply the meta-slopes developed for this study. This is an assumption that allows for estimation of a reduction target. We fully acknowledge that using meta-slopes developed for the Inner Danish waters is an assumption associated with uncertainties, both because the indicator is defined differently, and due to the ecosystem differences mentioned by the expert panel. We are presently in the process of initiating a project focusing on the finalization of a mechanistic biogeochemical model for the North Sea that can consolidate reduction targets in these water bodies.

***Q:* A serious weakness of the report is that the input data basis is not sufficiently presented. Tables are lacking that show spatially resolved values for present and past atmospheric deposition, spatially resolved emission data from land, concrete concentrations in all rivers and estuaries for both N and P, and hydrographic data (e.g. % freshwater, residence time, tide, depth) for all systems. The lack of area specific data does not allow a critical evaluation of regional MAI nor a comparison with data and results from other countries. The panel would greatly appreciate if such a table could be produced, preferably electronically.**

A: We apologies for the lack of input data. The evaluation report has focused on models and methodologies behind the Danish MAIs. We have prepared and sent a xls-spread-sheet with the data we have readily available.

Detailed questions

Page	Report	Question
16		It seems formally strange to attribute F as "index" when it is a dimensional quantity (dimension L^3/T^2) and it does not appear very logical to divide runoff with residence time, that is, wouldn't a longer residence time imply larger runoff influence? Why not use a more straightforward parameter around specific freshwater content: f=R/(Q+R) = (Sm – S)/Sm
	A: The applied F index was adopted from the Dahl et al. 2005 and has originally been used to make a typology for Danish marine waters as part of the initial Danish implementation of WFD. It has not been a part of the present study to evaluate or revise the F index.	
17	Fig. 3.2	Type 1 subtypes represent different nitrogen and phosphorus regimes, ranging from the quite Baltic Sea influenced to quite North Sea influenced, should perhaps this be taken into account in the model validation? On the other hand, the number of Type 1 areas that are both critically dependent on Danish nutrient inputs and significantly deviating from GES are probably limited.
	A: The verification presented in the scientific documentation summarizes the model results between the different water body regimes ranging from eutrophied closed estuaries to open waters. While working with the different models they have all been calibrated/verified separately applying a number of monitoring stations across the model domains. During this process, we did include monitoring stations scattered across the Danish marine waters, but for the scientific documentations we did not provide more information on the differences between the open waters. In Annex 1 we did include a few examples for various Type 1 water bodies, Figure 34 to Figure 45.	
20 / 58	*"In addition to the Danish land*-based loadings, the mechanistic models also include N and P loadings at a regional scale, i.e. loadings to the entire Baltic Sea, and *atmospheric deposition, see chapter 7."* and P 58: *"An* important input to the setup of the mechanistic models is the external supply of nutrients. Apart from Danish land-based nutrient loadings, the mechanistic models include nutrient input to the Baltic Sea from other countries and atmospheric deposition. In section 4.2, Danish land-based nutrient loadings and atmospheric deposition are described, both based on data from the Danish monitoring programme *DNAMAP."*	In shallow waters, assumptions with respect to atmospheric deposition input can be crucial and potentially allow a manipulation of the MAI. Was the deposition data spatially resolved? If not, how was it taken into account in the model? Were gradients between land and sea taken into account? Which atmospheric N fractions were considered as bio-available in the model and how were they calculated? Was the

		atmospheric input of P fractions considered, as well?
	A: As mentiond earlier, the atmospheric model was executed with a grid resolution of 16 km in order to handle the land-sea gradients, and the model has different deposition velocities for the different surface types (different forest types, different crops, grass etc, and open water) in order to handle gradients in the deposition velocities to the different surface types. It is only the total deposition to open waters (with a spatial resolution of 16 km), which have been used as input to the mechanistic biogeochemical model. The model entails a chemical model including the transformation from NO and NO2 to NHO3 and nitrate aresols, as well as the chemical transformation of NH3 to NH4 (via acids like H2SO4 og HNO3), and through a dry and wet deposition those nutrients are allocated to different surface types, like the water surface of the Baltic Sea. Thus, output of the model is two species of nitrogen for wet and dry deposition, respectively. After summation per species of wet and dry deposition, the data is applied as input in the biogeochemical modelling. Atmospheric deposition of P was not considered.	
24	Time series of observatio ns (including Kd)	How was Kd measured?
	A: Before 1998, water transparency was in general measured as Secchi depth by the counties. The exception was monitoring performed by the National Environmental Research Institute, Denmark, that had CTD equipped with light sensors (4π PAR). After 1998, the counties monitoring vessels were also equipped with CTD's including sensors for surface light and 4π PAR censors on the CTD. Kd was estimated from light readings every 0.2 m according to common technical guidelines (Kaas and Markager, 1998, in Danish). For the current project, the Secchi depth data were converted to Kd-values as described in Murray and Markager (submitted to Frontiers in Marine Science). This analysis is based on more the 61,000 paired observations and Secchi depth and Kd and take into account the seasonal and spatial variability in the Kd*Sd factor.	
31	*"only time series with a minimum of 15 years were used"*	What is the statistical justification? How much data are omitted?
	The length of the time series determines the number of data points used for the regression. Statistical theory dictates that the confidence of a regression decreases with the number of data points as the residual degree of freedom decreases, and similarly when the number of explanatory variables increases. As a rule of thumb, the residual degree of freedom is calculated as the number of observations – (number of explanatory variables + 1) *(though dependent on the collinearity in the explanatory variables in PLSR)*. There is no objective way to determine the minimum number of data points and the choice of 15 years as threshold value was based on our experience with the data analysis. This is a compromise between representing as many waterbodies as possible and avoiding poorly monitored waterbodies, with few observations and hence increased uncertainty in the coefficients or erroneously selected variables.	
32	*"… refrained from doing so" (Log transformation)*	Are data normally distributed?
	A: Not all data are normally distributed, nor is this required in the PLSR assumptions.	

32	*"daily values gained from interpolation were used to construct monthly average values"*	Do you have a statistical reference for this procedure?
	A: The problem arises from the fact that the observations are unevenly distributed in time. More samples have been taken during the growing season, in order to monitor the environmental situation more closely during the most critical time of the year. In some cases, technical problems or conditions at sea have caused loss of data. Basically this is just a way to make a time weighted mean. The interpolation method has been widely used and has been used for these types of data for decades. We are aware of other techniques, e.g. GLM-procedures. However, we have found that such procedures generate other problems (e.g. GLM does not account for variable month lengths).	
33	*"… we defined the following rules for predictor variables"*	Do you have statistical criteria or a reference for this? There are robust & complete time series analysis theories and methodologies available
	A: The first part is a question, and, no, we do not have a reference. The rules have been developed for the specific purpose of this analysis, given the nature of the data and the aim of the analysis. We have sought to explain the reasoning behind the rules in the report (p. 33). As there are no specific question to these, we find it difficult to go into a more detailed explanation. We are familiar we other approaches, e.g. Box-Jenkins Time-series analysis and Fourier transformations. However, we have found that they are less suited for the problem. This is not to say that they cannot be applied. However, it was not possible to do a systematic comparison of several methodological approaches with the framework of this project.	
37	*"The half saturation coefficients (Ks) for phosphorus and nitrogen were chosen to be 0.2 uM and 2 uM"*	What was the final weight of this exercise in the selection of variables?
	A: We have not assessed the weight of this for the variable selection.	
41		Why did you not estimate error variances and confidence limits which are preconditions for evidence based, adaptive management, policy and decision making?
	A: We have applied several statistical measures in order to quantify the applicability of the models to describe the indicators (Chla, Kd etc.) of which e.g. the empirical standard error of the cross-validated model (RMSECV) can be easily converted to variance and confidence limits. However, there is no formal parametric way of calculating error variance for the slope in PLSR nor for the final model. The variance of the PLSR slopes could perhaps be estimated empirically using jack-knifing but the computational time to do this for approx. 100 models poses a challenge. Likewise there is no formal way of calculating confidence limits for the MAI estimates. Instead we have used ensemble modelling and sensitivity tests as a surrogate for a more formal assessment of model uncertainty and to assess the consequences of uncertainty in input parameters (status values, target values and models) for the MAI estimate. Hence, because of the complexity in the calculations, which hinder formal uncertainty analysis, we have used other measures in order to quantify the uncertainty related to the models and MAI calculations.	

42	*"… quantification of autocorrelation , this effect was not included in the models"*	Your justification conflicts with your observation of significant autocorrelation, doesn't it?
	A: We are not sure what the evaluation panel mean by this question. The occurrence of autocorrelation, particular for TN and TP is described in the paragraph om page 42 and a possible explanation. In essence; yes, autocorrelation occur in the time series for TN and TP, and means that the slope in the models are underestimated. However, at present, the time series are too short to quantify this and therefore we refrain from including this in the models. In relation to this and to some of the other questions raised about the technical details, we kindly ask the evaluation panel to consider that the framework for the analysis was subject to tight constrains in time and resources. Thus, the task was to obtain the best possible estimates under these conditions and with the data available.	
52		Calculation of Chl-a and KD is critical in this study. Thus, more information on how Chl-a is calculated from phytoplankton carbon and on the optical model parameterization relating model state-variables to KD would be interesting.
	A: This is be available in the DHI references forwarded to you as part of the answers. See fx. Section 3.1. and 3.3.11 in DHI (2014).	
59	*„However, an important difference between the national* data and the data adopted by DHI for the mechanistic modelling is the resolution in time. Whereas the national data are reported on an annual basis, the data used for the modelling were provided on a daily basis, both for water *discharges and nutrient loadings."*	How was this done?
	A: The national yearly inventory of Q, N and P loads to Danish marine waters is based on a model taking precipitation and down-stream observations from a number of Danish catchments into account. For the national reporting, data are aggregated in both time and space to yearly loadings on a water body level. For this study, we received the data without this aggregation, meaning that we received daily catchment model output for this study. The daily data were delivered by AU.	
59	*„The loadi*ngs were estimated as discharges of total nitrogen (TN) and total phosphorus (TP). Since the mechanistic models differentiate between the different chemical forms (inorganic/organic, dissolved/particulate, nitrogen and phosphorous species), the data were subsequently transformed into nutrient forms required by the modelling. Through an assessment of available observations on nutrients in water discharged from Danish catchments, monthly relations between inorganic and organic nutrients were developed and applied to split TN and TP into an inorganic and an organic fraction. By combining TOC and COD/BOD observations, the organic part was further split to separate the organic nutrients into *the three forms adopted in the modelling process."*	Since the assumptions with respect of the model input are crucial for the later results, I like some clarifications. Am I right that you used (with respect to N) DIN and a part of TON as bio-available fractions in the model? How did you calculate it from biological and chemical oxygen demands (COD/BOD)? Did you take into account DON, as well? Was this calculated for every river separately or as an average for all Danish rivers? Could you give numbers about the relative share of each fraction for N and P?

	A: For sure, the assumptions with respect of the model input are crucial for the later results, and we did spent some time trying to come up with a method for transferring river TN to the five different N-species included in the model (NH4, NOx, DN, CDON and LDON) and the 4 different P species (PO4, DP, CDOP and LDOP). During this process we developed an internal working paper describing the applied method. This is not an official document but we have included this paper as part of the answers to the expert panel.	
59	*„Hence, the data are those officially reported by the various* countries. Differentiation of TN and TP loadings was done *according to Stepanauskas et al. (2002).“ Stepanauskas et al. (2002): „We estimate that the input of summer riverine N* to the Baltic Sea consists of 48% dissolved inorganic N, 41% DON, and 11% particulate N. Corresponding values for phosphorus are 46%, 18%, and 36% of dissolved *inorganic P, DOP, and particulate P, respectively.“*	Is this the same approach that you used for Danish rivers? Stepanauskas et al. (2002) quantify DIN and DON and these are the fraction you used as input for all other Baltic areas, is this right? In some areas the model seems not to cover the entire coast and nutrient retention may take place between river input and onset of the model domain. How did you deal with it?
	A: The differences in how we handle N and P loadings from Danish respectively Baltic Sea rivers is described briefly in the attached internal working paper. It is correct that we do not resolve the entire coast – within the Danish waters we include the effects from retention for Odense Fjord, Roskilde Fjord and Limfjorden by applying local model results from the three estuaries in the IDW model. A number of the other estuaries are resolved in the IDW model but for the water bodies not resolved, and we do not include retention. For areas in the remaining part of the Baltic Sea, which is not resolved, we likewise do not include a retention.	
60	*“… data were lumped according to topology…” Fig. 7.6*	Did you calibrate models by water body? Evaluation by type does not reveal accuracy and precision of water body specific models, does it? Would it be possible to estimate error variances and confidence limits (e.g. 0,95) for water body specific models? What are the estimated mean, covariance and variance of model parameters and error variances of water body specific models?
	A: For the study, the models have been calibrated one-by-one and not lumped. Furthermore, the models have been calibrated according to specific monitoring stations and specific parameters for the individual stations. The lumping in e.g. Fig. 7.6. is an attempt to summaries the model across the different water body types. Examples of observations and model results are included in Annex 1: • Limfjord observations and model results: Figure 1 to Figure 13 • The Odense Fjord observations and model results: Figure 14 to Figure 23 • The Roskilde Fjord observations and model results: Figure 24 to Figure 33 • The IDW model observations and model results: Figure 34 to Figure 45	

	During the development of the scientific documentation, we did lump according to types trying to summaries the overall quality and highlighting the variation between the different types covered by the individual models. We did not estimate error variances and confidence limits but worked with BIAS and R^2.	
62	Skills of biogeochemical models	Is it true that all data was used for model calibration and that a model validation using an independent data set (year) was not carried out? In addition to regression coefficients demonstrating similar trends in model and data, can you also indicate that the actual values corresponded? Could you provide non-aggregated time series showing the model performance and data for concrete monitoring stations in comparison?
	A: It is correct that we used all observations available as part of the calibration process. Due to the limited amount of data available, setting data aside for verification would have left too few data for both calibration and validation. Therefore, with respect to the three estuarine models, identical data are used during the calibration process and the final verification. With regard to the IDW model, we did - in addition to monitoring data from inside the water bodies - calibrate the model against a number of monitoring stations outside the water body areas (open water stations), and these stations were not part of the final evaluation . When doing the more overall verification presented in the documentation report prepared for the panel, the majority of the monitoring stations/data included was not used for calibrations. Besides the regression coefficients demonstrating similar trends in model and data, we also included BIAS in the evaluation of the individual models. As requested by the expert panel, we have prepared some specific examples from the different models as part of this Q&As, these being presented in Annex 1 of this document (see figure numbers below). Not all monitoring stations in the different estuaries and open waters contain biogeochemistry and/or data covering all years. In Annex 1, we have included one monitoring station for each of the two models Odense Fjord and Roskilde Fjord, two stations for Limfjorden and three stations for IDW. The monitoring stations are chosen to reflect differences in water bodies. A criterion has been that data from the station cover a larger part of the modelled years. We have also included salinity and water temperature examples, but data has not necessarily been prepared for the exact same stations as for the biochemistry (not all data have been stored for all monitoring stations). The example figures included in Annex 1 are: Limfjord observations and model results: Figure 1 to Figure 13 The Odense Fjord observations and model results: Figure 14 to Figure 23 The Roskilde Fjord observations and model results: Figure 24 to Figure 33 The IDW model observations and model results: Figure 34 to Figure 45	

62	*"seasonal anoxia in these areas, inducing release of phosphorus from the sediments"*	Have the sorption-desorption on suspended sediment particles been taken into consideration?
	A: The estuarine models include sorption-desorption to inorganic sediment particles and hence is impacted by e.g. resuspension. The IDW model does not include the same interaction, as data on inorganic sediment for the IDW model area was insufficient for the model development.	
61		What is the point of validation based on water body Type? Type 1 waters seem to include as diverse areas as the ones inside the sills to rather marine areas in Kattegat, why not use the different sub-categories of Type 1, Figure 3.2 and Table 8.1? How is the aggregation done into Type averages in e.g. Figure 7.6? Just mean value water bodies (model/observed data)? The quantitative assessment (page 65-66) is done on monthly mean time-series. That implies a mixture of validation of seasonal cycle and inter-annual variability. At least for the non-open water Types, it would make sense to explicitly look at the interannual variability that probably gives more information on the model's capabilities of resolving the response to load reductions.
	A: We notice the point raised by the expert panel and have included some examples of modelled time series in Annex 1, Figure 34 to Figure 45. The model calibration has been performed on individual monitoring stations and not by aggregating for specific water body types. The aggregation in Figure 7.6 are mean values per water body (model and monitoring.	
76		The sediment pools are reduced for the reference simulation in the Baltic Sea and IDW based on literature values. But it is not explicitly stated whether this adaption resulted in a new quasi-steady-state in the model when forced with reference loads, which could be influential on several of the Type 1 water bodies. Is this the case?
	A: The model did not reach a new quasi-steady-state in all sub-areas of the IDW model after adopting the reductions in the sediment based on literature values. In some areas, the sediment seems to build up some additional nutrients pools following the reductions. We	

	do not observe a visual trend in surface concentrations but cannot rule out some long-term effects.	
77	You attribute the decrease due to UWWT in Copenhagen, population about 600 000	What management measures in the same time period have been implemented to treat the manure of the approx. 25million pigs? Each pig represents 3 person equivalents, so approximately 75 million people.
	A: We have not assessed any management measures – the comment to the figure is merely an observation and an explanation to the data representing the Northern Sound.	
84	*"In order to reduce the influence of model bias, we used …* ensemble model*s …" & "… most robust chlorophyll*-a *estimates were achieved using ensemble model"*	How can you justify this without proper error variance/uncertainty estimates?
	A: For both the mechanistic and statistical models error variance/uncertainty estimates would require e.g. Monte Carlo simulation and Jack-knifing which was not practically doable. Since we have no a priori knowledge of model performance in a low nutrient situation - a mean of the two models is believed to be the best estimate of the "true" value. It is also the most simple approach and the 'first choice' when no other information are available.	
87	*" … status values are converted into water body averages* by relating the observed status to the modelled status at the actual observation point and applying the ratio between the two (model and observation) to correct the modelled water *body average"*	Could you clarify? Are you correcting model results?
	A: We are using the model results to estimate a water body average based on the observations conducted in the specific water body. Hence, we assume the observations provide the best estimate of the status in the observation point, but use the model to extrapolate the observations to a water body average.	
89	*"The purpose of averaging … is to reduce uncertainty"*	Can you justify? Is average any more certain than either of the models?
	A: Averaging the reduction need for the individual indicators is believed to provide a more robust and precise estimate of MAI for a given water body since 1) we do not have a priori knowledge that one indicator is better than others and 2) consistently choosing the indicator with the highest reduction need (in order to ensure that all indicators reach GES) would increase uncertainty since it is an "extreme" value with an inherent higher risk of being influenced by both model - and observational errors.	
91		What is the method to estimate the weights? Could it be possible to use error variances of models as weights?
	A: Yes in principle it could be possible to use error variances as weights, and we acknowledge that this is a sound approach in an analysis with several parameters were the main difference is the uncertainty of the data/models. However, in this case the differences (outlined page 91-101) are not related to the uncertainty in the data but should reflect the formal – or juridical – difference; is the indicator intercalibrated in the WFD context? For these reason Kd and chlorophyll-a is given double weight. Secondly, the two indicators for	

	ecological signs of hypoxia are merged into one indicator, to obtain the same weight as the others.	
92	*"This choice is b*ased on our wish from a management perspective to emphasise intercalibrated indicators and has *no scientific basis"*	Does this mean the WFD intercalibration? Why does intercalibration not provide a scientific basis for the chosen indicators?
	A: Yes, what is meant by 'intercalibrated indicators' is the procedure in the WFD. However, this is not to say that the intercalibrated indicators are not sound indicators describing the environmental status. On the contrary, we find that both Kd and chlorophyll-a concentrations are highly relevant parameters. Our intentions with the sentence quoted above is just to emphasise that the 'double weight' to these parameters (Table 8.7) was argued in the fact that they are intercalibrated, which is a formal or juridical argument and not a scientific argument.	
97	*"we chose a half saturation coefficient (Ks) for nitrogen limitation of 2 µM"*	On what basis (published) was this concentration chosen? This is difficult for a mix of diatoms, cyanobacteria and dinoflagellates.
	A: The K_m-value (K_s is a mistake in the report, it is the half-saturation constant in a Michaelis-Menten kinetic there is meant, which usually is denoted K_m) is taken from the literature cited in the paragraph. This aspect of the analysis was published in Hydrology and Earth System Sciences (Hindsby et al. 2012). Different values for K_m can be found in the literature, but often in the range 1-3 µM DIN on system scale. It is clear that a K_m-value of 2 µM only is indicative as the affinity vary between species and also might depends if DIN is represented by ammonium or nitrate. It is also shown in the literature (¤ref.¤) that DON can be a source of nitrogen for phytoplankton. Rather than taxonomic group, size is clearly a factor that systematically affect K_m, with smaller cells having a higher affinity (¤ref.¤). This is also reflected in the observation for Danish marine areas, where cell size increase with chlorophyll concentration (Stæhr et al. 2004, Stæhr and Markager 2004). However, in a situation with low DIN-concentrations the phytoplankton community will adapt toward species with higher affinity – as stated – often smaller species. Thus, even that some types of phytoplankton clearly display much higher K_m-values; they will likely be replaced under nutrient poor conditions, meaning that a general value for K_m under 2 µM is meaningful for low DIN conditions. Although, we haven't made a complete sensitivity analysis, we expect that values in the range is 1-3 µM DIN will produce about the same results with respect to number of days with nutrient limitation, given that the change for high to low DIN concentrations in the spring is often occur within a few days. It should also be emphasized that we have not just used the K_m values as a rigid threshold but – as described in the report – we have analysed the relationship between the number of days with DIN and DIP concentration under these thresholds (2 and 0.2 µM respectively) and the observed Chl. a concentration with another K_m value the number of days would change, but so would the "break point" and hence the goal. Therefore only large changes in the K_m or a varying K_m would result in significant changes in MAI based on this supporting indicator alone.	
92 93 94 95	*"… Kd indicator … are assigned double weight"* *"… light attenuation indicator has beem giving double weight"* *"… we have transformed the estimated PLR values into categories when above 25 %"*	All of these choices sound arbitrary and cursory. Can you justify?

96 99 99	*"…due to the time constraints … we chose not to develop models" & "… the demand was assigned as 25 %.."* *"… values above one trigger a demand 25%"* *"we used categorization … as demonstrated in Table 8.7"* *"… the target values are rounded …"*	
	A: The 'choices' are not made 'cursory' but are all carefully considered expert judgements. The values are the results of discussions and careful considerations based on the 'raw' results from the analysis and our knowledge of the system and the development over the last decades combined with literature studies. We have sought to argue for the choices in section 8.3. As the question is not specific, we find it difficult to supplement this argumentation. To this point, we find it important to refresh the aim of the analysis; 'To give the best possible estimate of the reduction in press factors the can result in GES for Danish marine areas and hence compliance with the WFD. As the environmental statuses of Danish marine areas are quite far away from GES, the result can only be an estimate. The choices in question reflect our aim to find a balance and minimize the risk of both over and underestimation of the reduction in nutrient loadings.	
102		The scenarios have the basis that BSAP nutrient load reductions are implemented. These comprise of massive P-load reductions (e.g., 60% for Baltic Proper that eventually should lead to halving winter DIP concentrations there), but all published scenarios show that the response time is quite slow with typical e-folding time of say 20 years. How is this time-delay handled in the model?
	A: We have not assessed the time-delay. We have assessed the impact as we expect them to be over the coming decade. Our focus has been on evaluating the reduction targets that will ensure that Denmark fulfil Danish obligations towards WFD in all water bodies given that the loadings from other countries comply with BASP.	
111		It is surprising that massive load reductions to Baltic Sea do not give more response to basin 217. The export of phosphorus from the Baltic proper should decrease substantially given that DIP concentrations should be reduced to 50% of present day concentrations in BSAP. Could you explain?
	A: Since the adaptation of the BSAP significant reductions (although especially the Baltic Proper still lack significant P reductions) in both N and P loads have been implemented and observed (HELCOM 2011). However, when assessing the impact in observed concentrations of both DIN, DIP, TN and TP in the Baltic Proper, and even more evident in the Arkona Basin and Bornholm Basin (HELCOM 2013), the reductions in concentrations does not reflect the reductions in loads. Hence, scenario results behind BSAP show that eventually significant	

	reductions in e.g. DIP is expected, but the observations indicate that this could be impacted by climate and, as mentioned by the expert panel, time-lag. Our modelling has the BASP loading reductions as a prerequisite and the modelling result provide the expected impact of reductions for the coming decade (and not several decades). In this period, the model do not indicate a significant impacts on e.g. summer chlorophyll-a and Kd even when implementing BSAP fully.	
124	*"With respect to the North Sea water bodies, the data basis* does not support the methodology described for mechanistic model-based meta model since biogeochemical modelling was not included in the study. However, GES has not been reached in any of the Danish water bodies in the North Sea and Skagerrak, and an approach taking limitation and differences into account has therefore been developed	What is meant by this statement? It is unclear
	A: As we did not develop a mechanistic biogeochemical model for the North Sea, we could not assess the reduction targets in a similar way as for the water bodies in the Kattegat and Baltic Sea area. However, since the status assessment showed there is a need for improvement of the environmental status (GES is not reached), we developed a method (a meta-model) to circumvent the missing data from biogeochemical modelling. As mention in the general Q&As we are working with the Danish EPA to develop a biogeochemical model for the RBMP 2021-2027.	
125	The described approach is subject to uncertainty.	Can the uncertainty be expressed in a way that it is easily understood by decision makers and stakeholders?
	A: This is basically a very interesting question. Especially, as it is extremely difficult for all parts to understand what to do about the uncertainties.	
129	*"…95% confidence interval at +/- 13.5 % reduction"*	What can you say about model error variances and confidence limits based on the comparison of mechanistic and statistical models? Is this 13.5% the overall confidence interval of loading reduction?
	A: The 13.5% is a calculated confidence interval for the percentage load reduction. This can be translated to a confidence interval of approx. +/- 20% on the estimated MAI. This is not a result of a "traditional" uncertainty analysis which is not possible to perform, but a result of ensample modelling in 11 water bodies covered by both a statistical and mechanistic model.	
130		Does the observation that for area 44 the statistical model fails because it does not take regional reductions into account imply that the statistical approach would fail for all Type 1 water bodies?
	A: We have developed statistical models for several Type 1 water bodies (including area 44), but not applied these in the final calculations of MAI (page 125 in report). This is because the statistical approach is best suited for estuaries were local nutrient loadings dominate over the nutrient exchange. Area 44 (Hjelm Bay) is on open bay on the south side of the island Møn. The location means that the catchment in Denmark is small and the connection	

	to the Western Baltic Sea is significant. Thus, it is an area were the statistical approach probably only could work when based on data for regional nutrient loadings or maybe not at all as the distance from nutrient loadings to effect is large. The statistical approach might work better for other Type 1 water bodies, especially those located in the inner Danish water where Danish land based loadings are more important. However, since the statistical models do not operate with non-Danish nutrient sources as explanatory variables we decided not to use this approach for Type 1 water bodies.	
141	*"the methods presented here basically violate the one*-out-all-out principle, which is defined when evaluating the ecological status and not when estimating measures to *ensure GES"; "When reductions based on chlorophyll*-a or Kd are averaged instead of choosing the maximum reductions,we do, in theory, not obtain GES for both *indicators"*	Is the method therefore WFD compliant? If not, what is necessary to make it WFD compliant? What management measures are necessary to obtain GES for BOTH indicators?
	A: Our hypothesis is the GES for both Kd and chlorophyll-a will be reached after reductions in nutrient loadings. However, the time scale in the response will probably be different, with chlorophyll-a reacting faster than Kd. The reason is that chlorophyll-a respond to the nutrient input to the system as well as the nutrient pool stored after decades with high loadings (see e.g. Jørgensen at al. 2014 and Knudsen-Leerbeck et al (2017). In contract, Kd is only for a small part related to the chlorophyll-a concentration (see e.g. Pedersen et al. 2014 and Carstensen 2013) but closely correlated with the total amount of organic matter in the systems. This difference in response has also been described in Timmermann et al. 2010. The use of an average reduction target instead of the calculated maximum reduction target will, at least formally, indicate that at least one parameter will not reach GES but it will also reduce the risk of overestimating the reduction target. Therefore, we suggest an adaptive management strategy where the effects of the suggested nutrient reductions (based on average, instead of maximum reduction targets) are evaluated after some years and then, if necessary, additional measures can be implemented. It should be noticed that even if the light climate is sufficient for eelgrass (i.e. the Kd indicator has reached GES), it is very likely that the official indicator "eelgrass depth limit" has not reached GES.	
141		It is stated that the basis is to obtain GES in 2027. This is fine, but it also has consequences on how to handle effects from regional reductions (BSAP), see the comment above on scenarios (page 102). It would be relevant to discuss the time aspect already in the beginning of the report as well, because we know the ecosystem responds slowly, and differently across the water bodies.
	A: We acknowledge that the ecosystem responds slowly, and especially the expected impacts from the actions taken according to BSAP and the Gothenburg Protocol. We believe that the estimated reduction targets should be seen as the reductions needed to obtain GES in Danish water bodies, but we cannot guarantee that observations will support this in 2027.	
142	*"… focused on reducing uncertainties,* for instance by *averaging … and applying a type*-specific approach	You lose information at the same time. Can you guarantee reduction of

		uncertainties without proper statistical error analysis, that is, comparison on error variances of models based on actual and averaged data?
	A: Information might be lost when data is aggregated (averaged and/or type-specific) provided that the uncertainty is low. However, this is not likely the case especially for estimating reference chlorophyll-a concentrations where the models are used far from the calibration area. Whenever individual values were considered too uncertain, we have prioritized robust (but aggregated) values with the risk of individual value deviating from the average/type-specific value.	
142	*"The* ensemble model results reveal good agreement *between the two very different model approaches …, thus indicating that the estimated MAIs are reliable"*	How can you say so without proper statistical error analysis?
	The rationale behind the statement is that since to independent methods obtain fairly similar predictions of MAI, it support the confidence in the result. It is not possible to perform traditional statistical error analysis on the MAI estimates. Instead we have used an ensemble approach when possible and although we cannot rule out the risk that the both models are biased or the error/uncertainty for each of the approaches is much higher than the difference between the approaches, it is highly unlikely ($P<0.0001$) that the two methods just by chance coincide for 11 independent areas and are highly correlated ($R2=0.85$).	

References

Almroth E & MD Skogen (2010) A North Sea and Baltic Sea Model Ensemble Eutrophication Assessment. AMBIO 39:59–69

Anker HT., 2016: Målrettet regulering – ekspropriation eller ej? moMentum+, 2, p. 32-34.

Björklund E, Styrishave B, Anskjær GG, Hansen M & B Halling-Sørensen (2011) Dichlobenil and 2,6-dichlorobenzamide (BAM) in the environment: What are the risks to humans and biota? Science of the Total Environment 409: 3732–3739

Borsuk, M.E., Stow, C.A., Reckhow, K.H., 2004. A Bayesian network of eutrophication models for synthesis, prediction, and uncertainty analysis. Ecol. Modell. 173, 219–239

Burson, A., M. Stomp, L. Akil, C. P. D. Brussaard, and J. Huisman 2016. Unbalanced reduction of nutrient loads has created an offshore gradient from phosphorus to nitrogen limitation in the North Sea. Limnology and Oceanography **61**: 869-888.

Canal-Verges, P., J. K. Petersen, E. K. Rasmussen, A. Erichsen, and M. R. Flindt 2016. Validating GIS tool to assess eelgrass potential recovery in the Limfjorden (Denmark). Ecological Modelling **338**: 135-148.

Carpenter, S. R., N. F. Caraco, D. L. Correll, R. W. Howarth, A. N. Sharpley, and V. H. Smith 1998. Nonpoint pollution of surface waters with phosphorus and nitrogen. Ecological Applications **8**: 559-568.

Carstensen, J., P. Henriksen, and A. S. Heiskanen 2007. Summer algal blooms in shallow estuaries: Definition, mechanisms, and link to eutrophication. Limnology and Oceanography **52**: 370-384.

Carstensen, J., and P. Henriksen 2009. Phytoplankton biomass response to nitrogen inputs: a method for WFD boundary setting applied to Danish coastal waters. Hydrobiologia **633**: 137-149.

Carstensen J, Krause-Jensen D, Markager S; Timmermann K & J Windolf (2013) Water clarity and eelgrass responses to nitrogen reductions in the eutrophic Skive Fjord, Denmark. Hydrobiologia 704: 293-309

Cloern, J. E. 2001. Our evolving conceptual model of the coastal eutrophication problem. Marine Ecology-Progress Series **210**: 223-253.

Dahllöf I, Mogensen BB, Bossi R & I Jensen (2008) Forekomst af herbicider i Nissum Fjord. Danmarks Miljøundersøgelser, Aarhus Universitet. 21 s. – Arbejdsrapport fra DMU nr. 244. http://www.dmu.dk/Pub/AR244.pdf

Dennison, W. C. 1987. Effects of Light on Seagrass Photosynthesis, Growth and Depth Distribution. Aquatic Botany **27**: 15-26.

Devault AD and H Pascaline (2013). Herbicide Impact on Seagrass Communities, Herbicides - Current Research and Case Studies in Use, Dr. Andrew Price (Ed.), InTech, DOI: 10.5772/55973. Available from: https://www.intechopen.com/books/herbicides-current-research-and-case-studies-in-use/herbicide-impact-on-seagrass-communities.

DHI (2016) DHI 3 Algae and Sediment Model. ECO Lab Template. Scientific Description. DHI Water Environment Health, Hørsholm, Denmark, 134 pp.

Duarte, C. M. 1991. Seagrass Depth Limits. Aquatic Botany **40**: 363-377.

Duarte, C. M. 1995. Submerged Aquatic Vegetation in Relation to Different Nutrient Regimes. Ophelia **41**: 87-112.

Duarte, C. M., N. Marba, D. Krause-Jensen, and M. Sanchez-Camacho 2007. Testing the predictive power of seagrass depth limit models. Estuaries and Coasts **30**: 652-656.

Duarte, C. M. 2009. Coastal eutrophication research: a new awareness. Hydrobiologia **629**: 263-269.

Flindt, M. R., E. K. Rasmussen, T. Valdemarsen, A. Erichsen, H. Kaas, and P. Canal-Verges 2016. Using a GIS-tool to evaluate potential eelgrass reestablishment in estuaries. Ecological Modelling **338**: 122-134.

Hansen, J. W. Marine områder 2015. NOVANA. 208. 2016. Aarhus Universitet. Videnskabelig rapport fra DCE-Nationalt Center for Miljø og Energi. Ref Type: Generic

HELCOM (2011) The Fifth Baltic Sea Pollution Load Compilation (PLC-5). Baltic Sea Environment Proceedings No. 128. Helsinki Commission, 217 pp. http://www.helcom.fi/Lists/Publications/BSEP128.pdf.

HELCOM (2013) Approaches and methods for eutrophication target setting in the Baltic Sea region. Baltic Sea Environment Proceedings No. 133. Helsinki Commission, 134 pp.

Herbert, R. A. 1999. Nitrogen cycling in coastal marine ecosystems. Fems Microbiology Reviews **23**: 563-590.

Hrustic, E., R. Lignell, U. Riebesell, and T. F. Thingstad 2017. Exploring the distance between nitrogen and phosphorus limitation in mesotrophic surface waters using a sensitive bioassay. Biogeosciences **14**: 379-387.

Jorgensen, L., S. Markager, and M. Maar 2014. On the importance of quantifying bioavailable nitrogen instead of total nitrogen. Biogeochemistry **117**: 455-472.

Kemp, W. M., W. R. Boynton, J. E. Adolf, D. F. Boesch, W. C. Boicourt, G. Brush, J. C. Cornwell, T. R. Fisher, P. M. Glibert, J. D. Hagy, L. W. Harding, E. D. Houde, D. G. Kimmel, W. D. Miller, R. I. E. Newell, M. R. Roman, E. M. Smith, and J. C. Stevenson 2005. Eutrophication of Chesapeake Bay: historical trends and ecological interactions. Marine Ecology-Progress Series **303**: 1-29.

Koch, E. M. 2001. Beyond light: Physical, geological, and geochemical parameters as possible submersed aquatic vegetation habitat requirements. Estuaries 24: 1-17.

Knudsen-Leerbeck, H., M. Mantikci, M. Bentzon-Tilia, S. J. Traving, L. Riemann, J.L.S. Hansen, S. Markager (2017) Seasonal dynamics and bioavailability of dissolved organic matter in two contrasting temperate estuaries Biogeochemistry, 134, 217-236, /doi:10.1007/s10533-017-0357-2

Krause-Jensen D, Carstensen J, Nielsen SL, Dalsgaard T, Christensen PB, Fossing H & MB Rasmussen (2011) Sea bottom characteristics affect depth limits of eelgrass Zostera marina. MEPS 425: 91-102.

Krause-Jensen D & MB Rasmussen (2009) Historisk udbredelse af ålegræs i danske kystområder. Danmarks Miljøundersøgelser, Aarhus Universitet, 38 p. (Faglig rapport fra DMU; No. 755).

Kaldy JE (2014) Effect of temperature and nutrient manipulations on eelgrass Zostera marina L. from the Pacific Northwest, USA. JEMBE 453: 108–115

Lyngsgaard, M. M., S. Markager, and K. Richardson 2014. Changes in the vertical distribution of primary production in response to land-based nitrogen loading. Limnology and Oceanography **59**: 1679-1690.

Markager, S., L.M. Storm & C.A. Stedmon (2006) Limfjordens miljøtilstand 1985 til 2003. Sammenhæng mellem næringsstoftilførsler, klima og hydrografi belyst ved empiriske modeller. Report no. 577, *National Environmental Research Institute,* Denmark. www.dmu.dk.

Maycock D, Crane M, Atkinson C and I Johnson (2010) Proposed EQS for Water Framework Directive Annex VIII substances: glyphosate (For consultation). Water Framework Directive - United Kingdom Technical Advisory Group (WFD-UKTAG); SNIFFER 25 Greenside Place Edinburgh EH1 3AA Scotland

Miljøstyrelsen (2017) Bekæmplesesmiddel statistik for 2015. Behandlingshyppighed og pesticidbelastning, baseret på salgsstatistik og sprøjtejournaldata. Orientering fra Miljøstyrelsen nr. 17, januar 2017

Møhlenberg, F., Petersen, S., A. H. Petersen, A.H. C. Gameiro (2007) Long-term trends and short-term variability of water quality in Skive Fjord, Denmark – nutrient load and mussels are the primary pressures and drivers that influence water quality. Environ Monit Assess 127: 503-521

Negri AP, Flores F, Mercurio P, Mueller JF & CJ Collier (2015) Lethal and sub-lethal chronic effects of the herbicide diuron on seagrass. Aquatic Toxicology 165: 73–83

Nielsen, S. L., K. Sand-Jensen, J. Borum, and O. Geertz-Hansen 2002a. Depth colonization of eelgrass (Zostera marina) and macroalgae as determined by water transparency in Danish coastal waters. Estuaries **25**: 1025-1032.

Nielsen, S. L., K. Sand-Jensen, J. Borum, and O. Geertz-Hansen 2002b. Phytoplankton, nutrients, and transparency in Danish coastal waters. Estuaries **25**: 930-937.

Nielsen LW & Dahllöf (2007) Direct and indirect effects of the herbicides Glyphosate, Bentazone and MCPA on eelgrass (Zostera marina). Aquatic Toxicology 82: 47–54

Nixon, S. W. 1995. Coastal Marine Eutrophication - A Definition, Social Causes, and Future Concerns. Ophelia **41**: 199-219.

Pedersen, M. F. 1995. Nitrogen Limitation of Photosynthesis and Growth - Comparison Across Aquatic Plant-Communities in A Danish Estuary (Roskilde Fjord). Ophelia **41**: 261-272.

Pedersen, M. F., and J. Borum 1996. Nutrient control of algal growth in estuarine waters. Nutrient limitation and the importance of nitrogen requirements and nitrogen storage among phytoplankton and species of macroalgae. Marine Ecology-Progress Series **142**: 261-272.

Pedersen, O., T. Binzer, and J. Borum 2004. Sulphide intrusion in eelgrass (Zostera marina L.). Plant Cell and Environment **27**: 595-602.

Pedersen, T.M., K. Sand-Jensen, S. Markager & S. L. Nielsen (2014) Optical changes in a eutrophic estuary during reduced nutrient loadings. Estuaries and Coast 37, 880-892. doi: 10.1007/s12237-013-9732-y.

Petersen, M. E., M. Maar, J. Larsen, E. F. Moller, and P. J. Hansen 2017. Trophic cascades of bottom-up and top-down forcing on nutrients and plankton in the Kattegat, evaluated by modelling. Journal of Marine Systems **169**: 25-39.

Pogson M & P Smith (2015) Effect of spatial data resolution on uncertainty. Environmental Modelling & Software 63: 87-96

Pulido Pérez C & J Borum (2010) Eelgrass (Zostera marina) tolerance to anoxia. JEMBE 385(1-2): 8-13.

Ralph, P. J., M. J. Durako, S. Enriquez, C. J. Collier, and M. A. Doblin 2007. Impact of light limitation on seagrasses. Journal of Experimental Marine Biology and Ecology **350**: 176-193.

Riemann, B., J. Carstensen, K. Dahl, H. Fossing, J. W. Hansen, H. H. Jakobsen, A. B. Josefson, D. Krause-Jensen, S. Markager, P. A. Staehr, K. Timmermann, J. Windolf, and J. H. Andersen 2016. Recovery of Danish Coastal Ecosystems After Reductions in Nutrient Loading: A Holistic Ecosystem Approach. Estuaries and Coasts **39**: 82-97.

Roca G, Alcoverro T, Krause-Jensen D, Balsby TJS, van Katwijk MM, Marba N, Santos R, Arthur R, Mascaró O, Fernández-Torquemada Y, Pérez M, Duarte C & J Romero (2016) Response of seagrass indicators to shifts in environmental stressors: A global review and management synthesis. Ecological Indicators 63: 310-323.

Ryther, J. H., and W. M. Dunstan 1971. Nitrogen,Phosphorus, and Eutrophication in Coastal Marine Environment. Science **171**: 1008-&.

Smith, V. H. 2003. Eutrophication of freshwater and coastal marine ecosystems - A global problem. Environmental Science and Pollution Research **10**: 126-139.

Smith, V. H., S. B. Joye, and R. W. Howarth 2006. Eutrophication of freshwater and marine ecosystems. Limnology and Oceanography **51**: 351-355.

Schmidt AL, Wysmyk JKC, Craig SE & HK Lotze (2012) Regional-scale effects of eutrophication on ecosystem structure and services of seagrass beds. Limnol Oceanogr 57(5). 1389–1402

Tamminen, T., and T. Andersen 2007. Seasonal phytoplankton nutrient limitation patterns as revealed by bioassays over Baltic Sea gradients of salinity and eutrophication. Marine Ecology Progress Series **340**: 121-138.

Thodsen, H., J. Windolf, J. Rasmussen, J. Bøgestrand, S. Larsen, H. Thornbjerg, and P. Wiberg-Larsen. Vandløb 2015. NOVANA. 206. 2016. Aarhus Universitet, DCE – Nationalt Center for Miljø og Energi. Videnskabelig rapport fra DCE - Nationalt Center for Miljø og Energi. Ref Type: Generic

Timmermann, K., S. Markager, and K. E. Gustafsson 2010. Streams or open sea? Tracing sources and effects of nutrient loadings in a shallow estuary with a 3D hydrodynamic-ecological model. Journal of Marine Systems **82**: 111-121.

Valdemarsen, T., P. Canal-Verges, E. Kristensen, M. Holmer, M. D. Kristiansen, and M. R. Flindt 2010. Vulnerability of Zostera marina seedlings to physical stress. Marine Ecology-Progress Series **418**: 119-130.

Weigel A.P., M.A. Liniger & C. Appenzeller. 2008. Can multi-model combination really enhance the prediction skill of probabilistic ensemble forecasts? Quarterly Journal of the Royal Meteorological Society 134: 241–260.

Annex 1

The Limfjord model

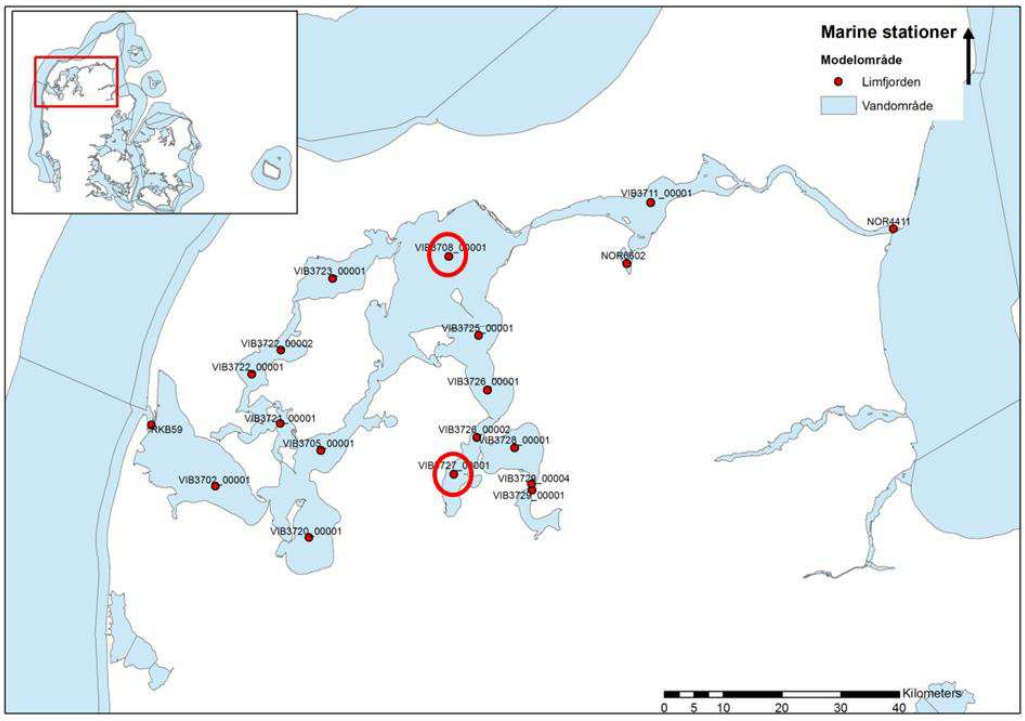

Figure 1: Monitoring stations applied within the Limfjord. Red dots indicate a monitoring station with at least 5 years of data within the period year 2000 to year 2012. Blue areas indicate the different Danish water bodies. The red circles indicate the locations of the time series included in this Annex.

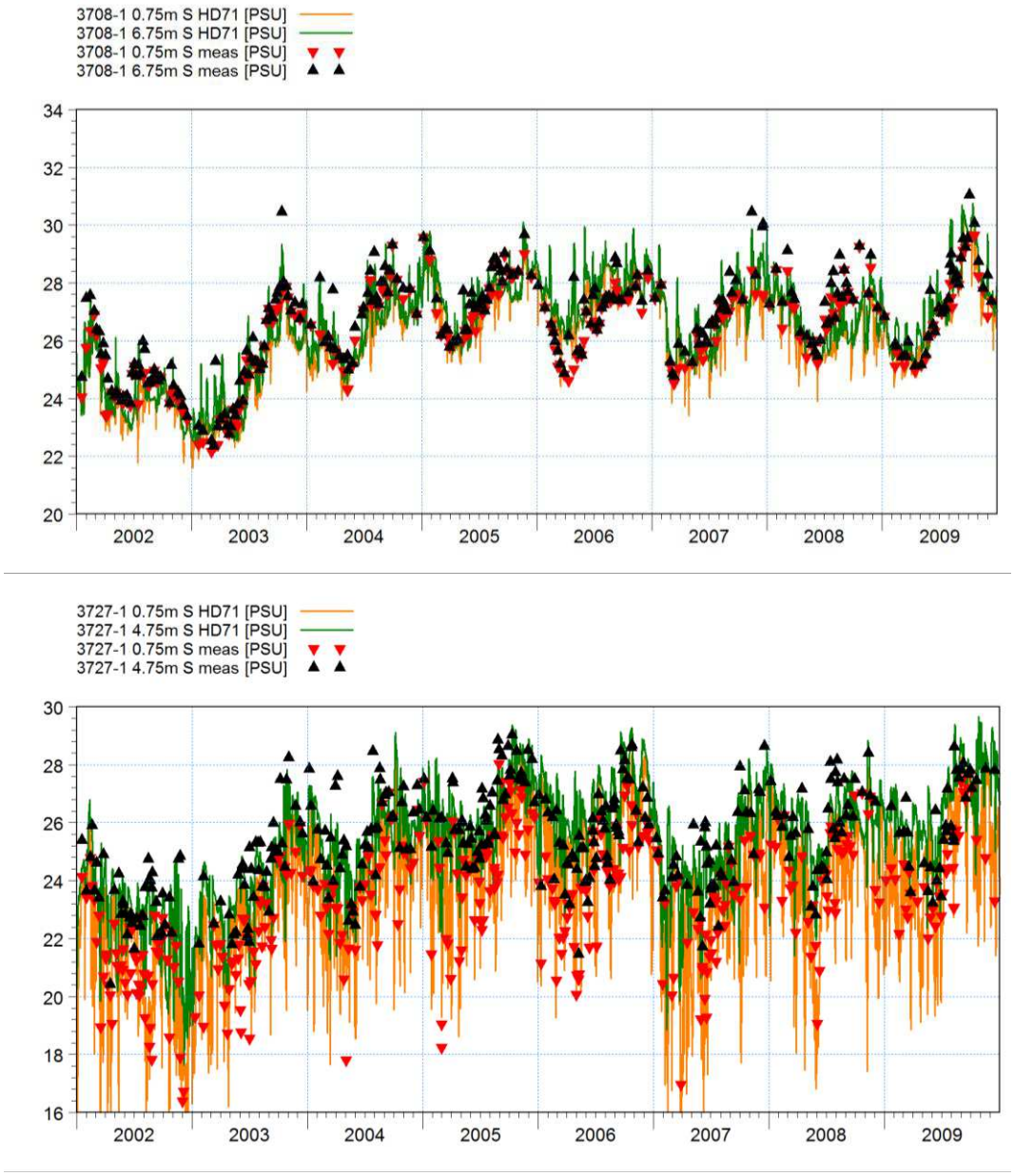

Figure 2: Comparison of measured surface (red markings) and bottom (black markings) salinity with modelled salinity at the surface (orange line) and at the bottom (green line) at 3708-1 and 3727-1.

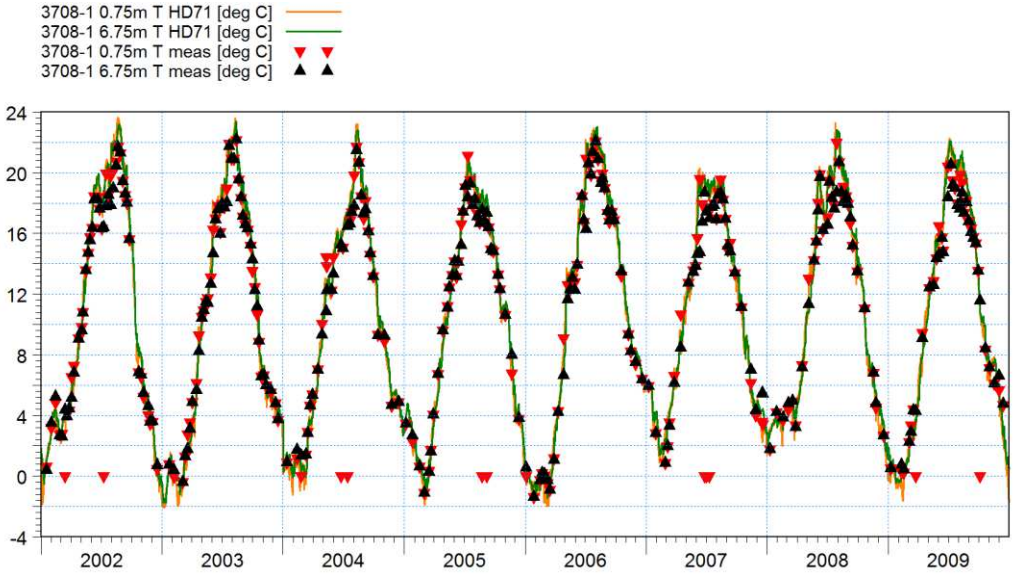

Figure 3: Comparison of measured surface (red dots) and bottom (black dots) water temperature with modelled water temperature at the surface (orange line) and at the bottom (green line) at 3708-1. Data from 3727-1 were not processed.

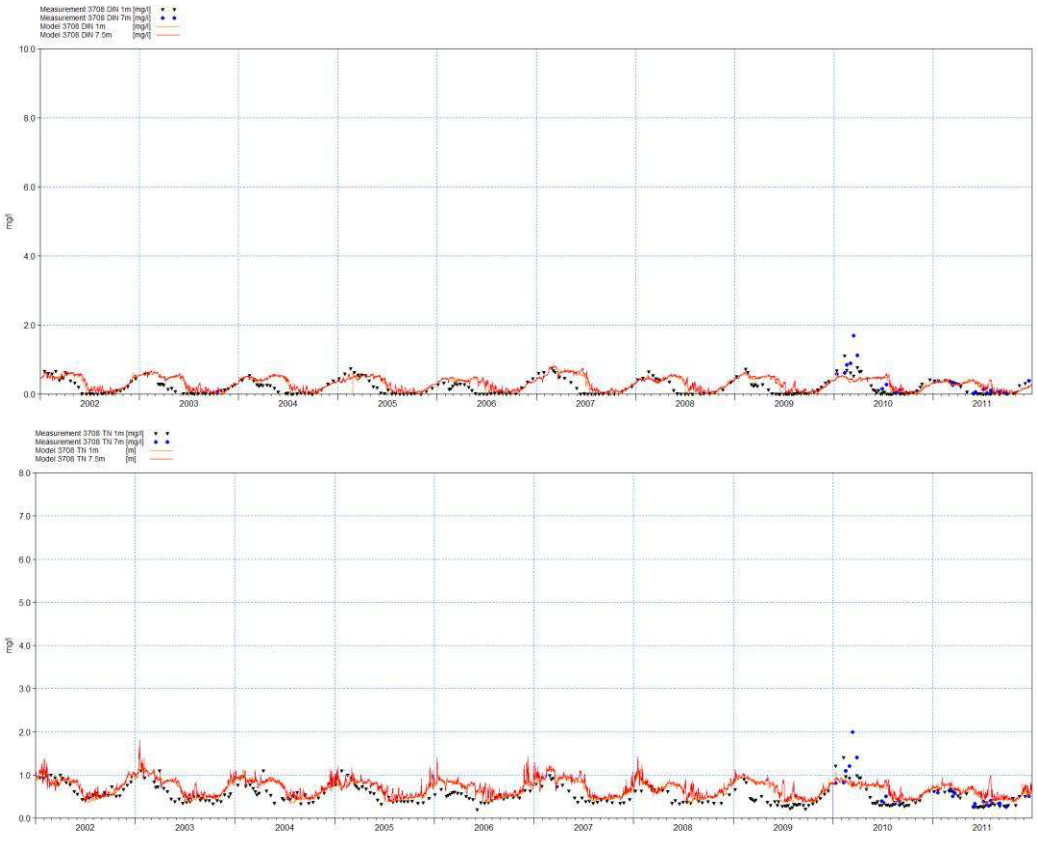

Figure 4: Measurements of nitrogen at station 3708-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface nitrogen (orange line) and bottom nitrogen (red line). At the top measurements and modelling results of DIN are shown, and at the bottom of TN.

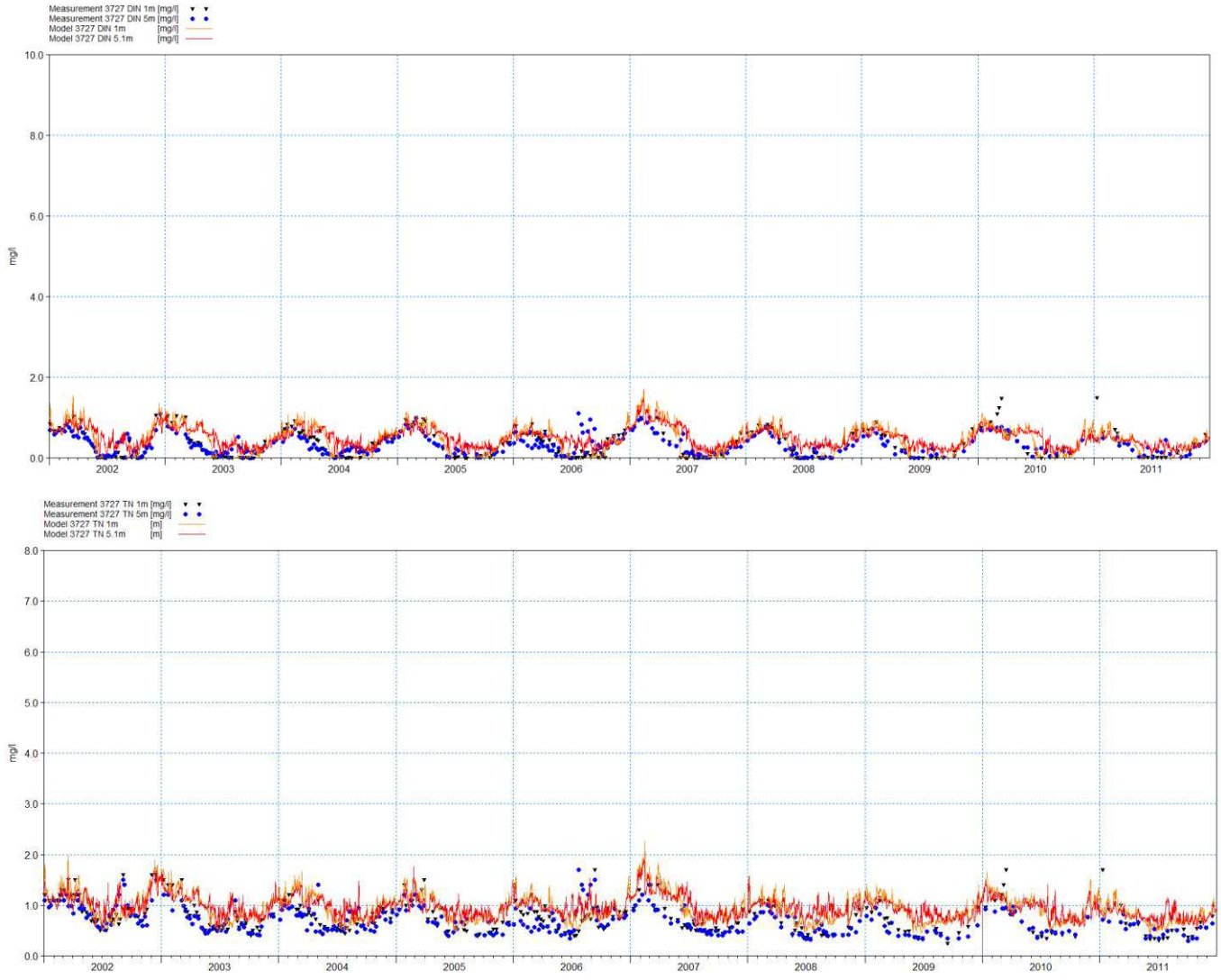

Figure 5: Measurements of nitrogen at station 3727-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface nitrogen (orange line) and bottom nitrogen (red line). At the top measurements and modelling results of DIN are shown, and at the bottom of TN.

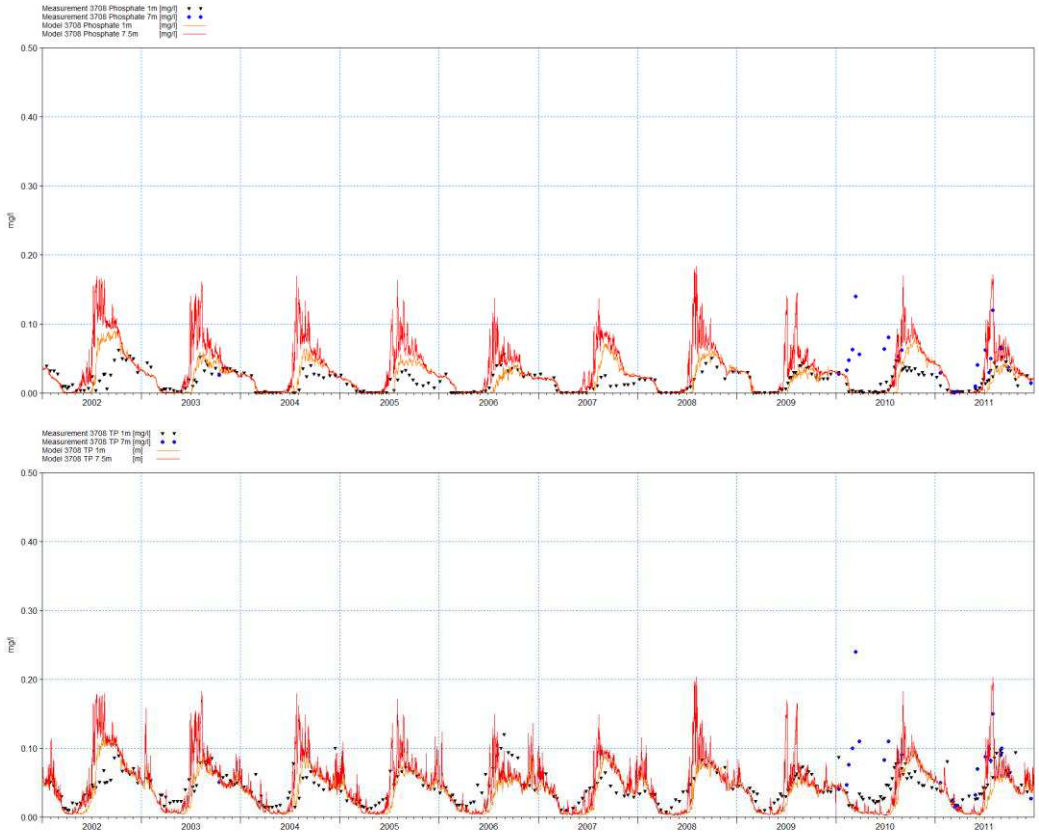

Figure 6: Measurements of nitrogen at station 3708-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface phosphorous (orange line) and bottom phosphorous (red line). At the top measurements and modelling results of DIP are shown, and at the bottom of TP.

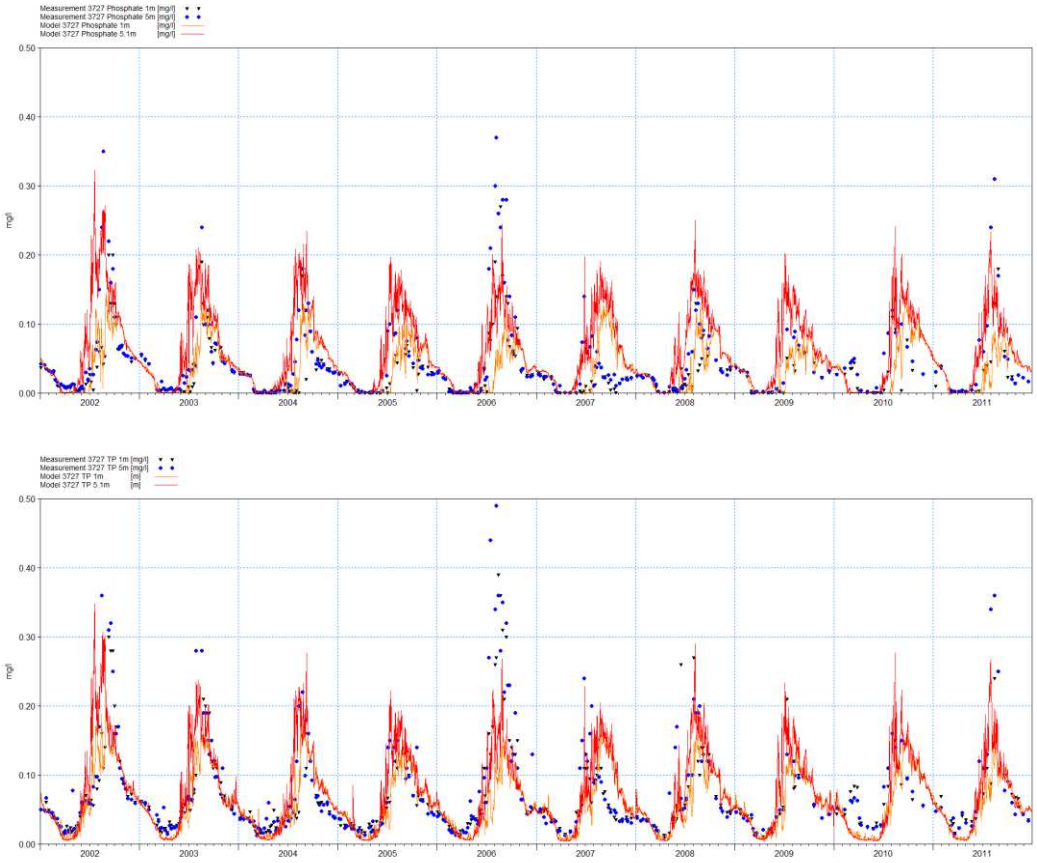

Figure 7: Measurements of nitrogen at station 3727-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface phosphorous (orange line) and bottom phosphorous (red line). At the top measurements and modelling results of DIP are shown, and at the bottom of TP.

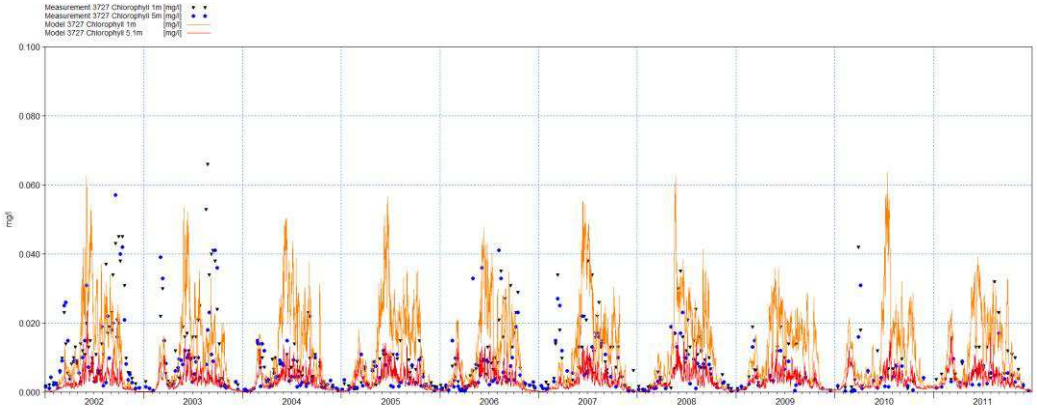

Figure 8: Measurements of chlorophyll-a at station 3727-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface chlorophyll-a (orange line) and bottom chlorophyll-a (red line).

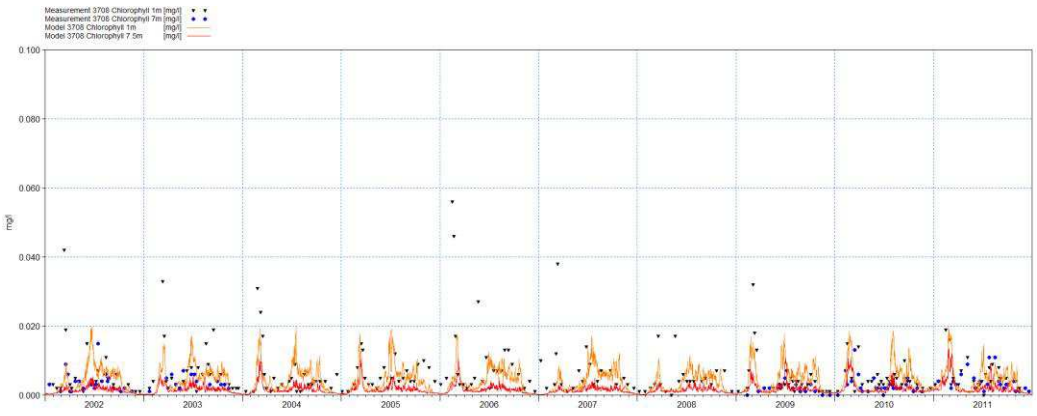

Figure 9: Measurements of chlorophyll-a at station 3708-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface chlorophyll-a (orange line) and bottom chlorophyll-a (red line).

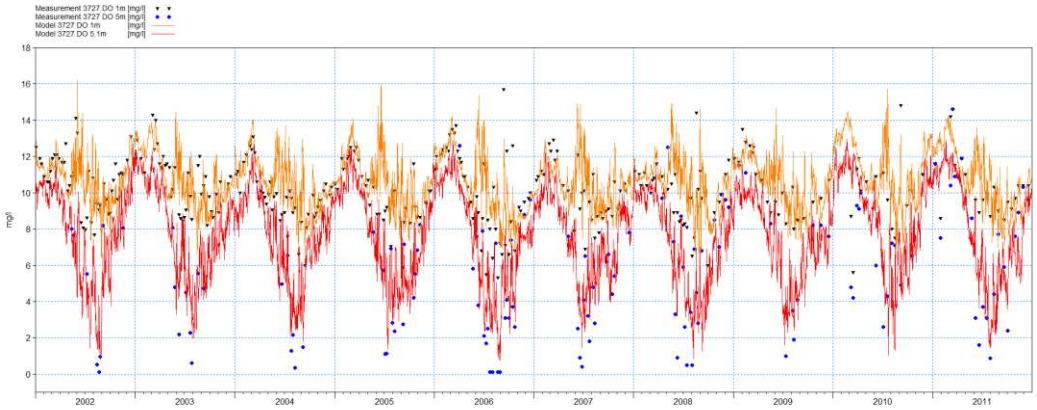

Figure 10: Measurements of dissolved oxygen at station 3727-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface dissolved oxygen (orange line) and bottom dissolved oxygen (red line).

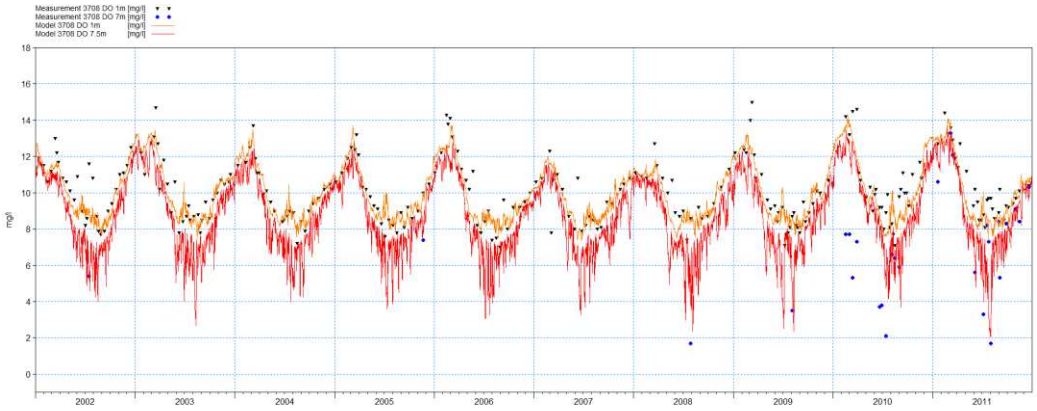

Figure 11: Measurements of dissolved oxygen at station 3708-1 in the surface (black markings) and bottom (blue markings) compared to modelled surface dissolved oxygen (orange line) and bottom dissolved oxygen (red line).

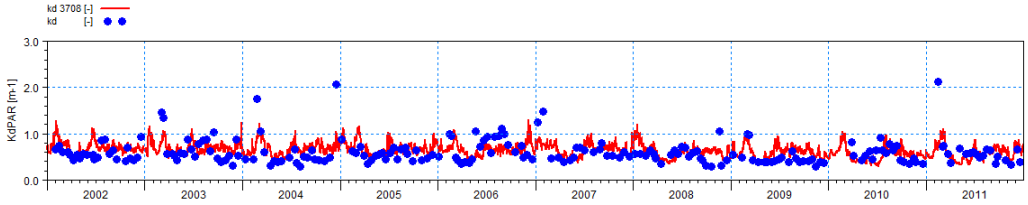

Figure 12: Measurements K_{dPAR} at station 3708-1 (blue markings) and modelled K_{dPAR} (red line).

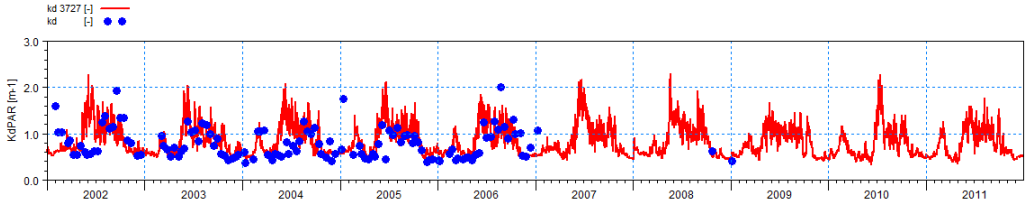

Figure 13: Measurements K_{dPAR} at station 3727-1 (blue markings) and modelled K_{dPAR} (red line).

Odense Fjord Model

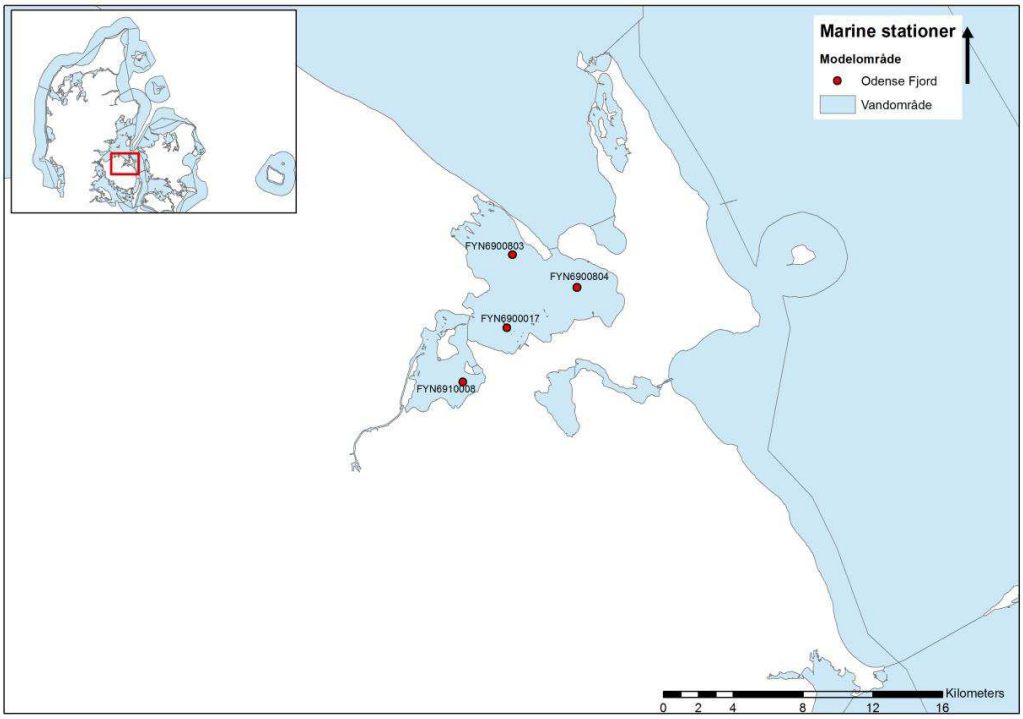

Figure 14: Monitoring stations applied for the Odense Fjord model performance. Biogeochemical data exists for two of the four stations in the map, and here we include the data from the central station FYN6900017.

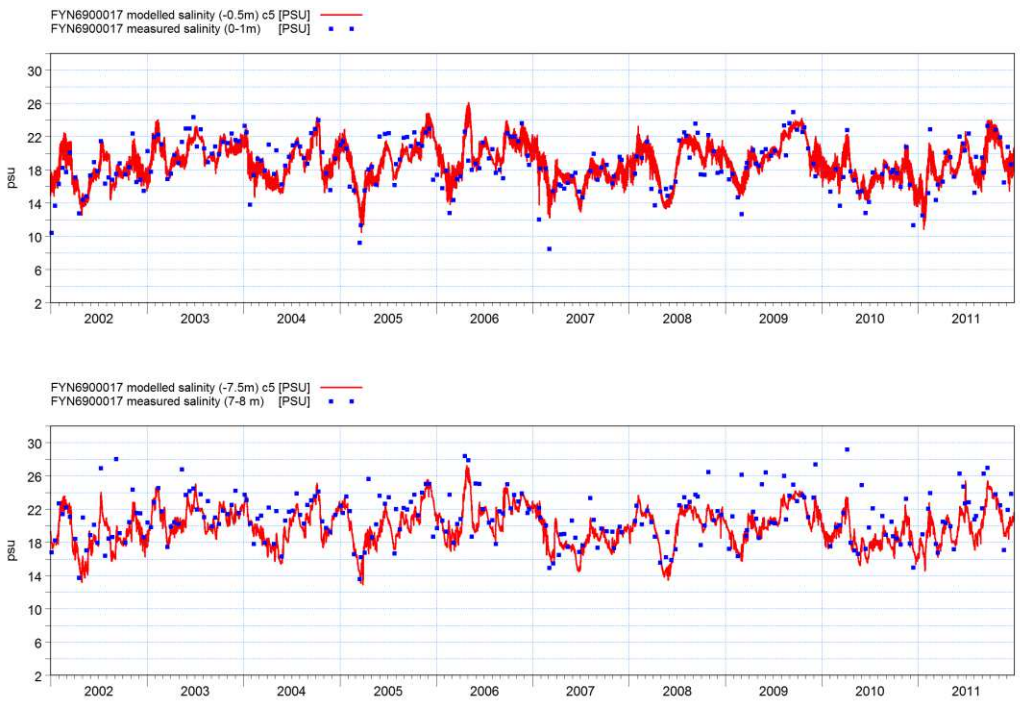

Figure 15: Comparison of measured and calculated salinity in the surface (upper) and on the bottom (lower) at station 69100017 in the outer fjord.

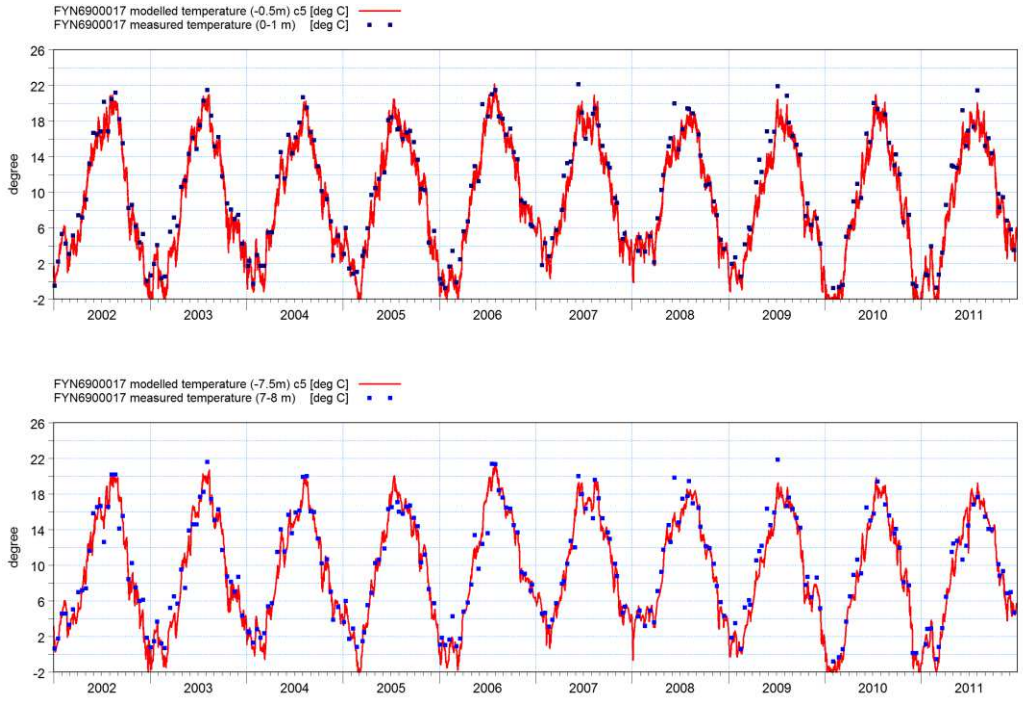

Figure 16: Comparison of measured and calculated water temperature in the surface (upper) and on the bottom (lower) at station 69100017 in the outer fjord.

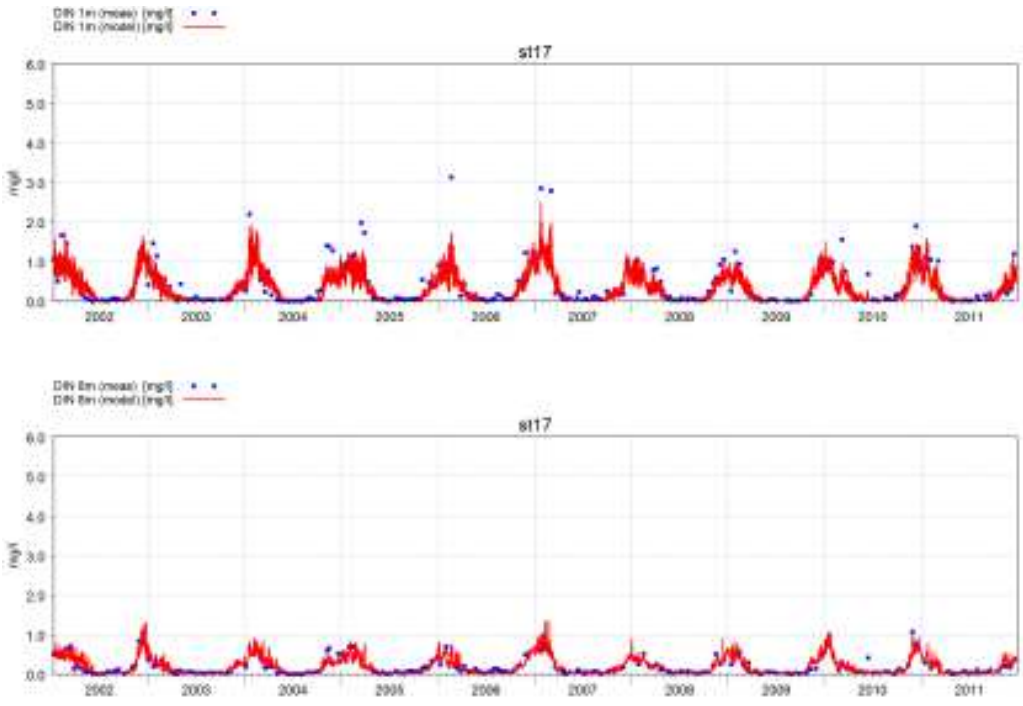

Figure 17: Measurements (blue markings) and model results (red lines) of DIN at station 6910017. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure.

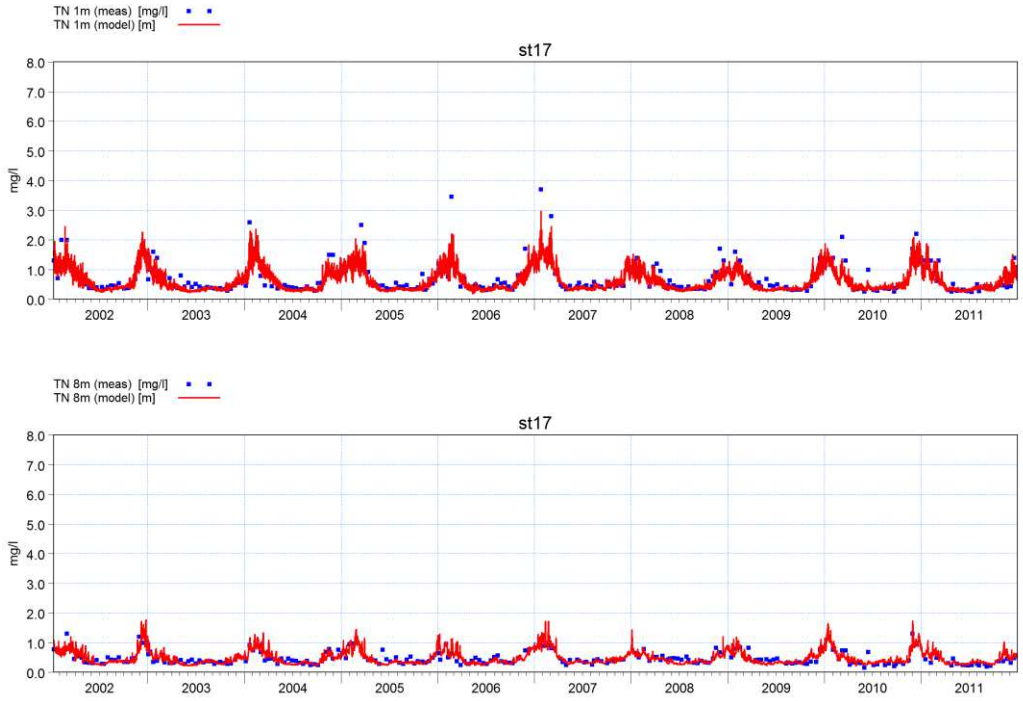

Figure 18: Measurements (blue markings) and model results (red lines) of TN at station 6910017. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure.

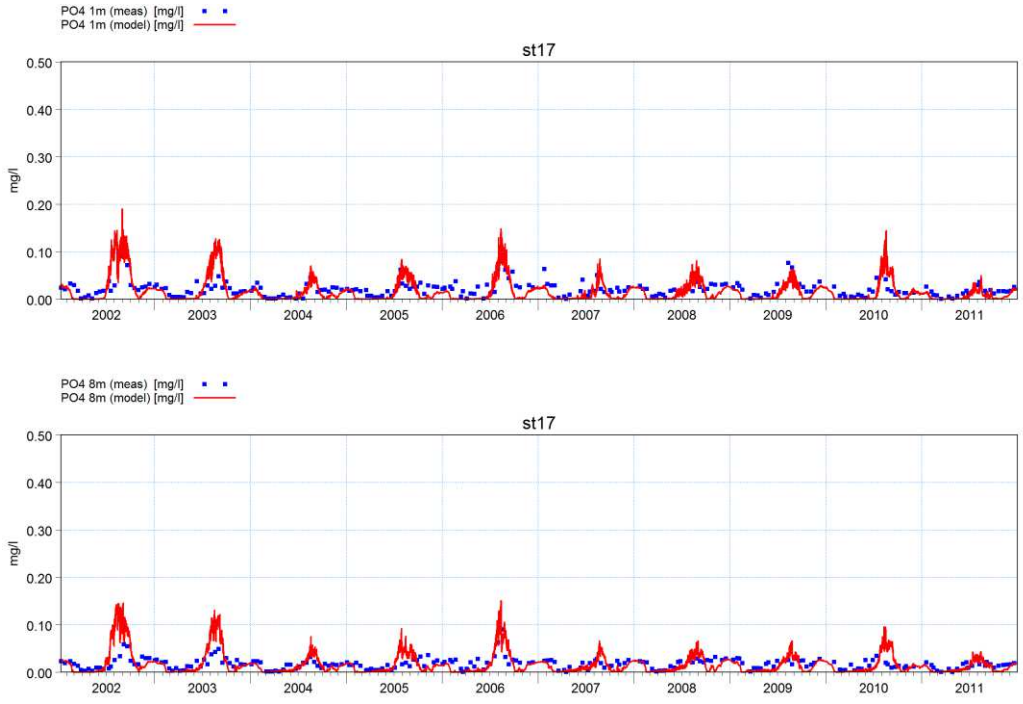

Figure 19: Measurements (blue markings) and model results (red lines) of DIP at station 6910017. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure.

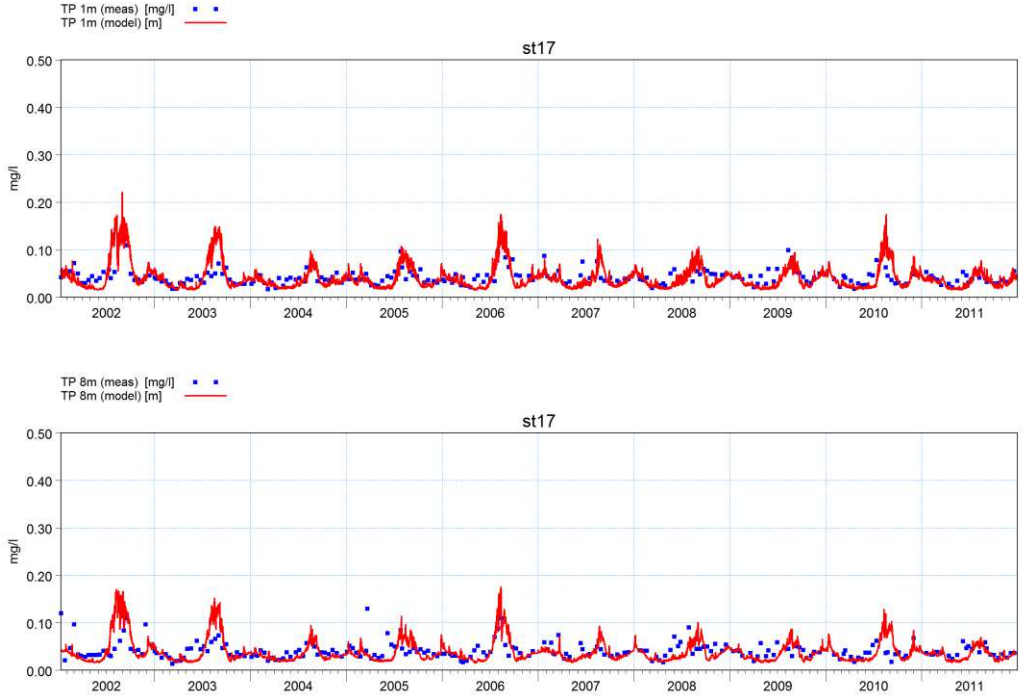

Figure 20: Measurements (blue markings) and model results (red lines) of TP at station 6910017. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure.

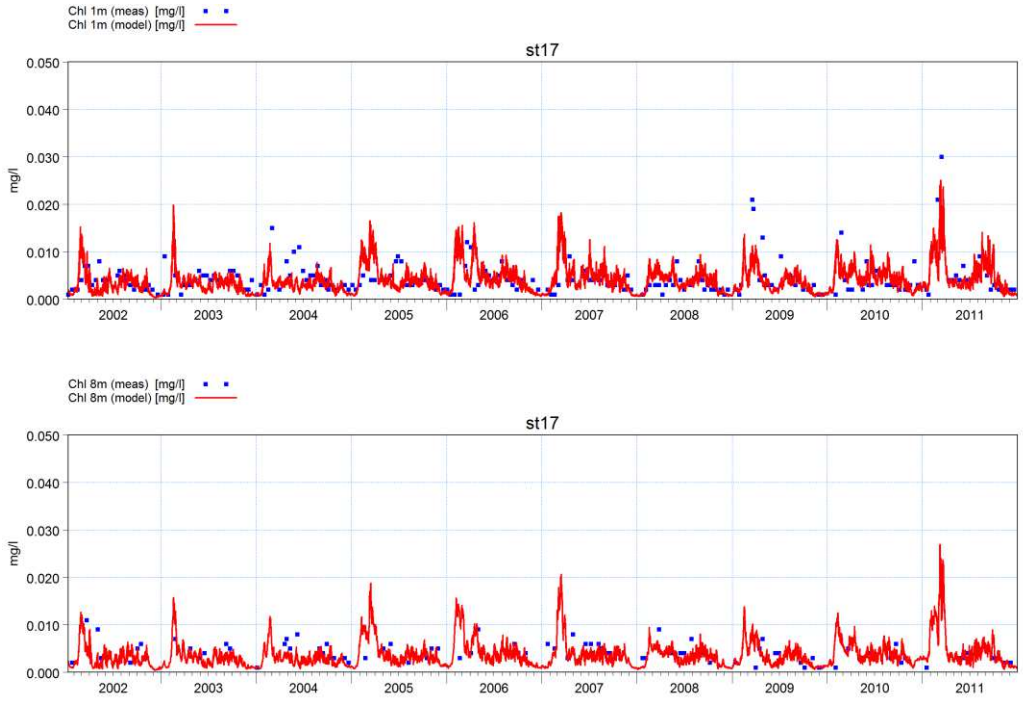

Figure 21: Measurements (blue markings) and model results (red lines) of chlorophyll-a at station 6910017. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure.

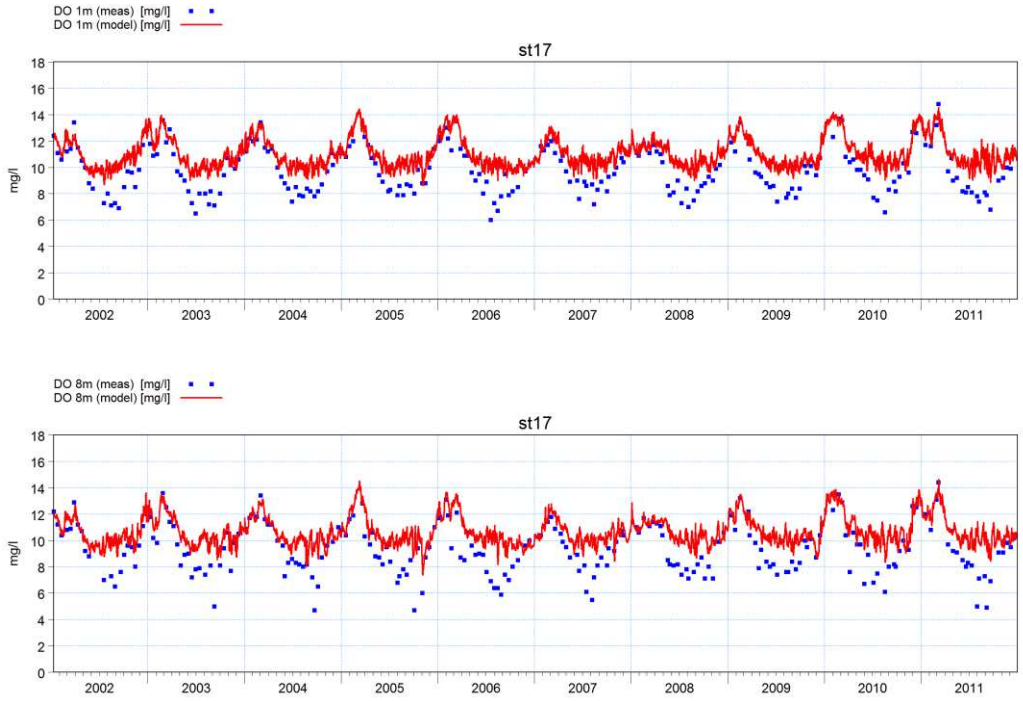

Figure 22: Measurements (blue markings) and model results (red lines) of dissolved oxygen at station 6910017. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure.

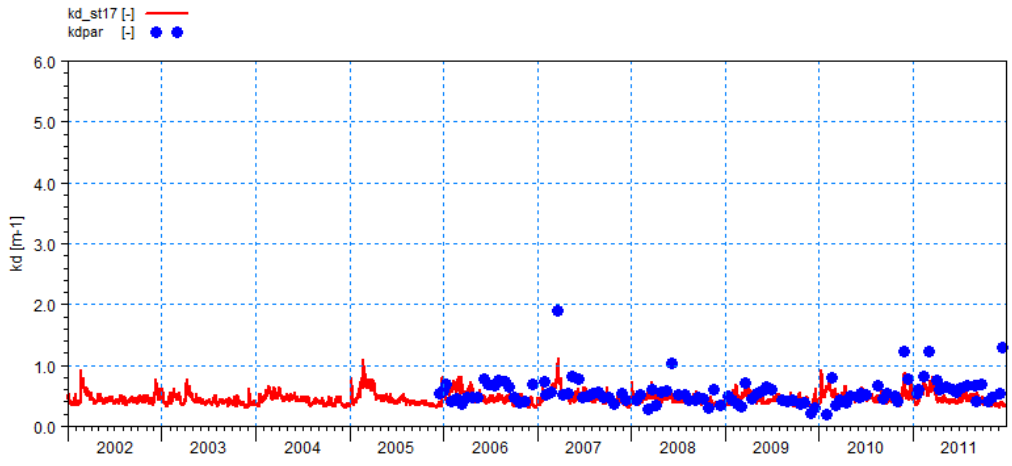

Figure 23: Measurements K_{dPAR} at station 6900017 (blue markings) and modelled K_{dPAR} (red line).

Roskilde Fjord Model

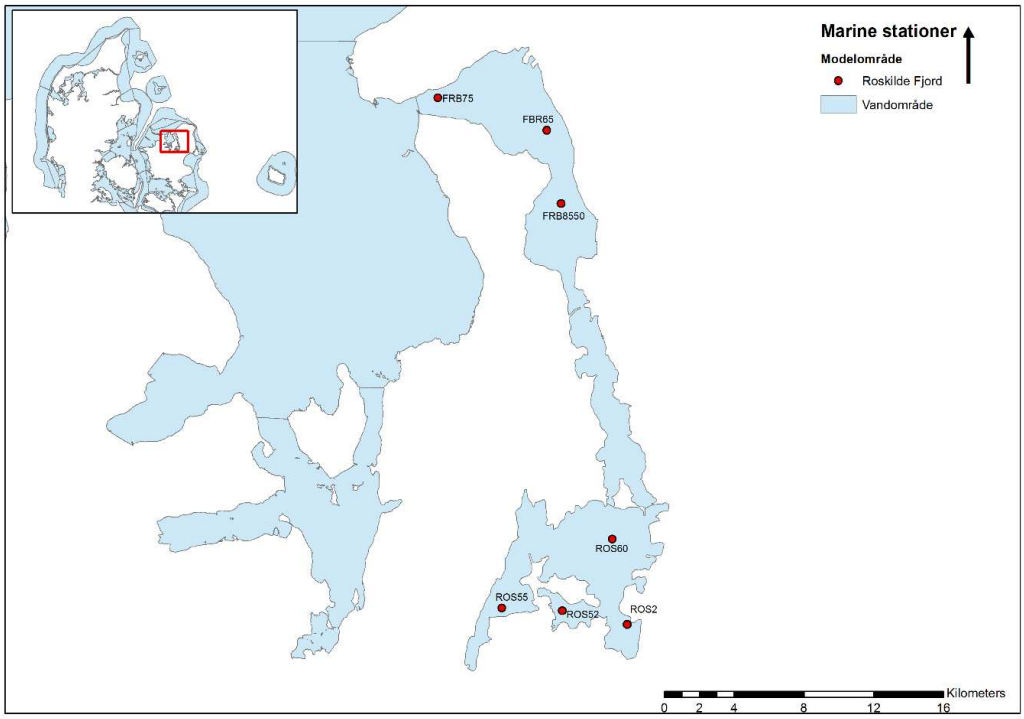

Figure 24: Monitoring stations applied for the Roskilde Fjord model performance. Continuous biogeochemical data exists for two of the stations in the map, and here we include the data from FBR65.

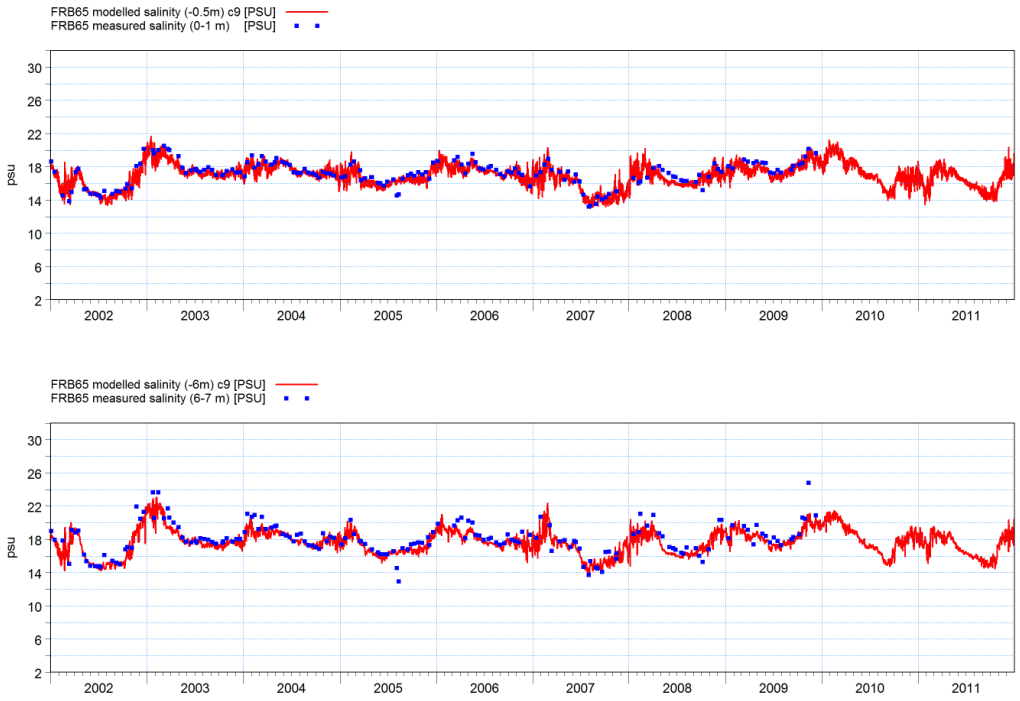

Figure 25: Comparison of measured and calculated salinity in the surface (upper) and on the bottom (lower) at station FRB65.

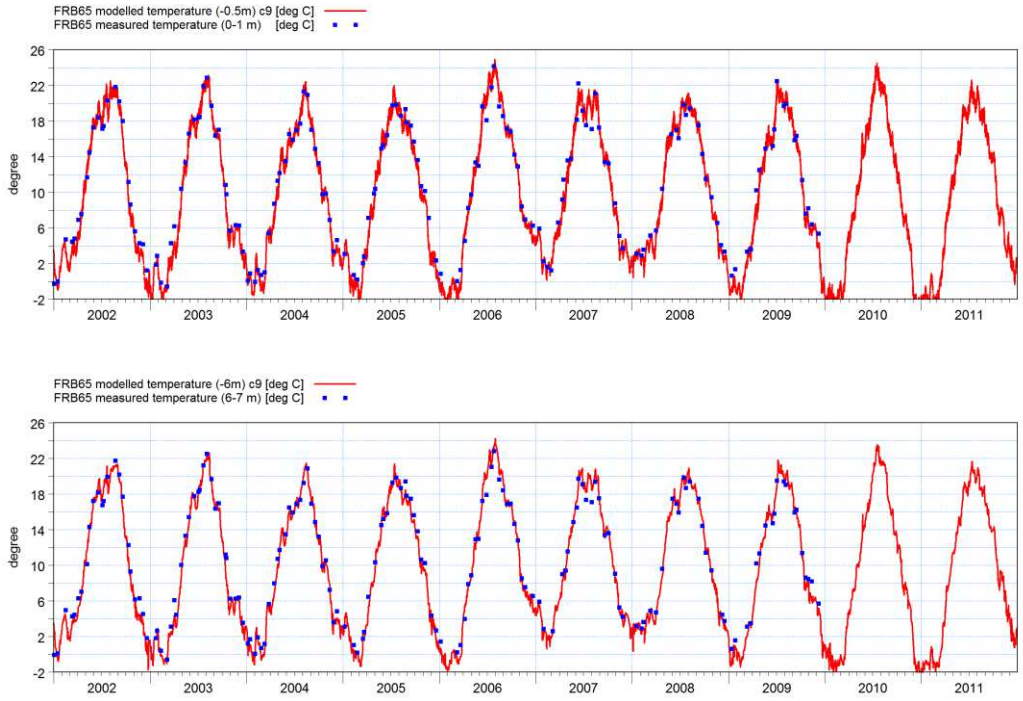

Figure 26: Comparison of measured and calculated water temperature in the surface (upper) and on the bottom (lower) at station FRB65.

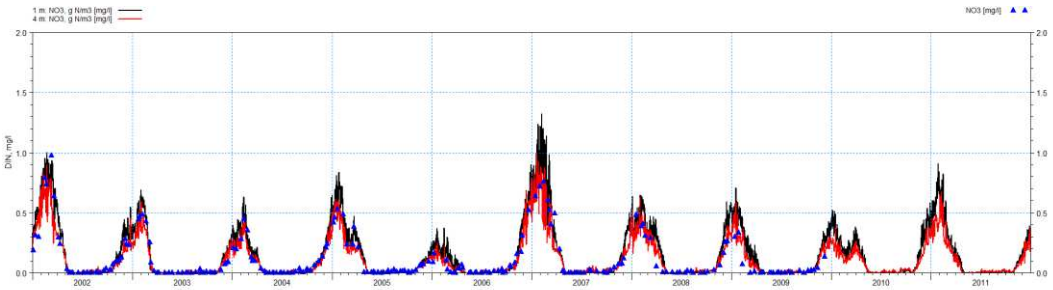

Figure 27: Surface measurements (blue markings) and model results (black line) of DIN at station FRB65. Red line indicate modelled bottom concentrations.

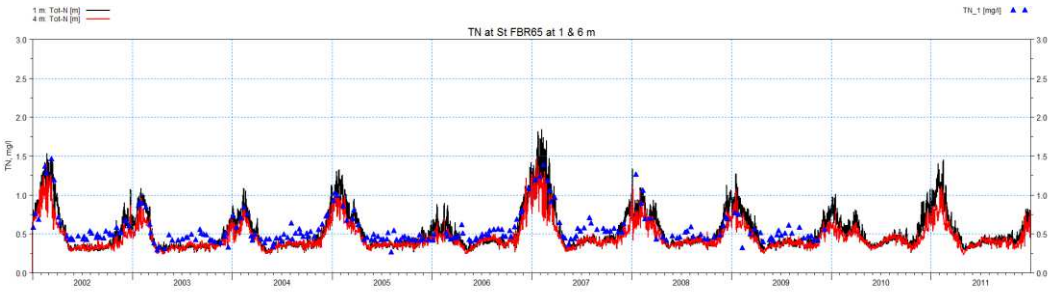

Figure 28: Surface measurements (blue markings) and model results (black line) of TN at station FRB65. Red line indicate modelled bottom concentrations.

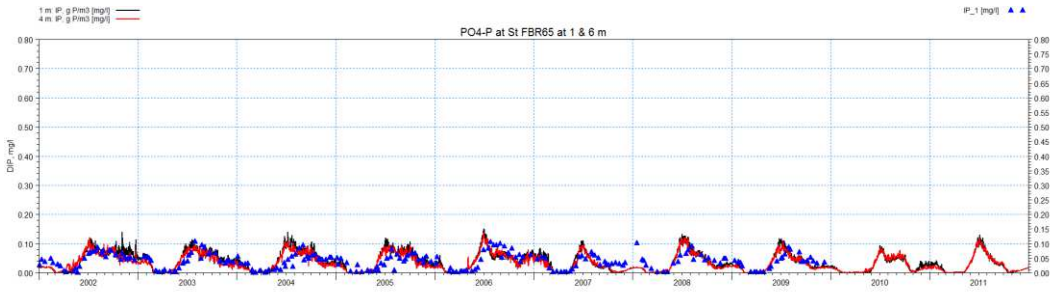

Figure 29: Surface measurements (blue markings) and model results (black line) of DIP at station FRB65. Red line indicate modelled bottom concentrations.

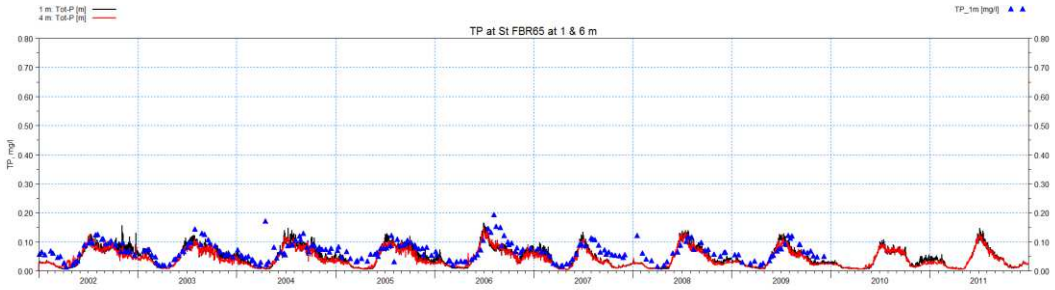

Figure 30: Surface measurements (blue markings) and model results (black line) of TP at station FRB65. Red line indicate modelled bottom concentrations.

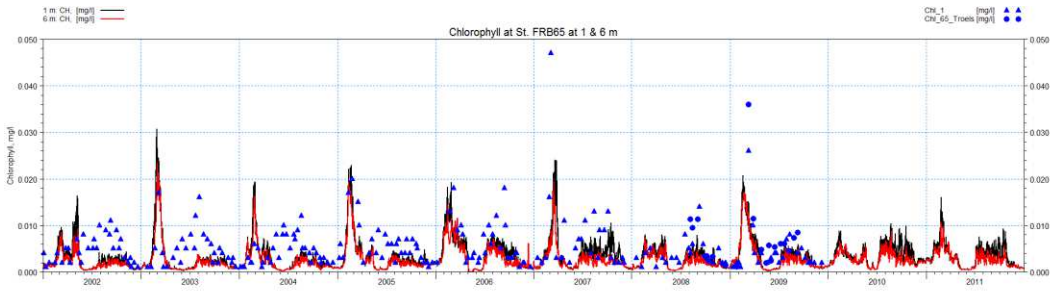

Figure 31: Surface measurements (blue triangles) and model results (black line) of chlorophyll-a at station FRB65. Red line indicate modelled bottom concentrations and blue circles indicate corresponding measured bottom concentrations.

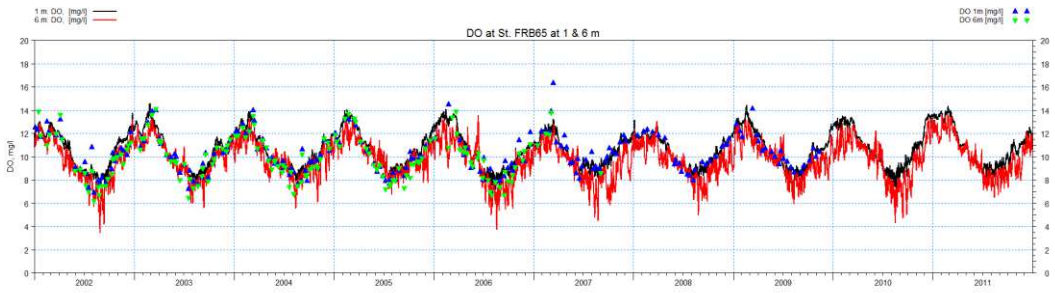

Figure 32: Surface measurements (blue markings) and model results (black line) of dissolved oxygen at station FRB65. Surface concentrations are shown in the top figure and bottom concentrations in the bottom figure. Red line indicate modelled bottom concentrations and green dots indicate measured bottom concentrations.

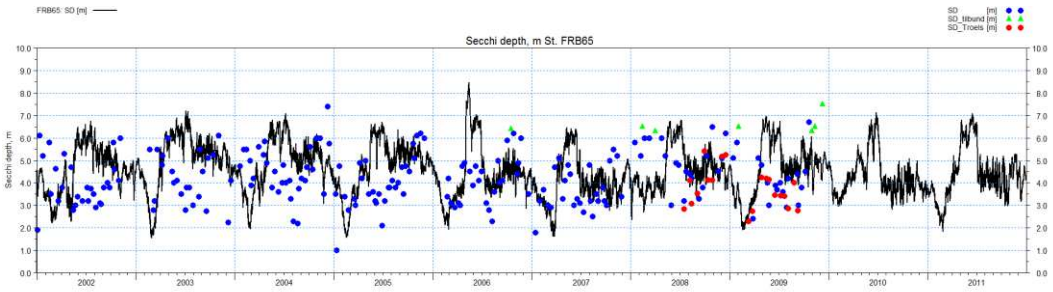

Figure 33: Measurements of Secchi disc depth at station FRB65 (blue and red markings – green markings show the water depth) and modelled Secchi disc depth (black line).

IDW Model

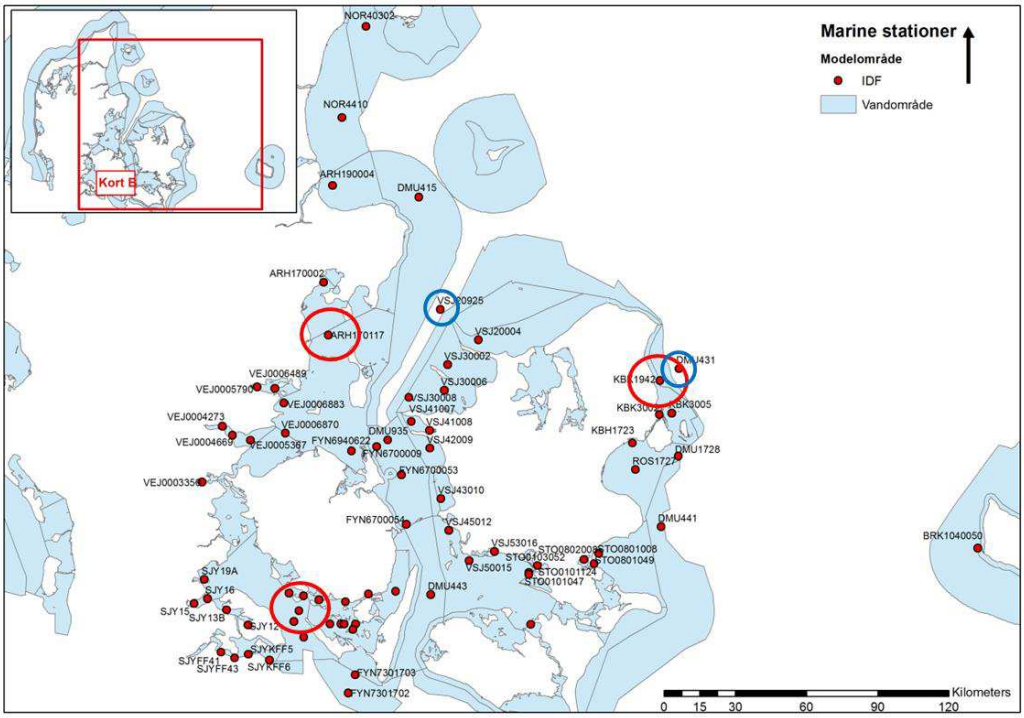

Figure 34: Monitoring stations applied for the IDW model performance analysis. Red dots indicate a monitoring station with at least 5 years of data within the period: Year 2000 to year 2012. Blue areas indicate the different Danish water bodies. Red circles show the biogeochemical monitoring stations included in this annex. Salinity and temperature are shown for the two station with blue circles. The differences between the locations of the salinity/temperature stations and biogeochemistry stations is due to which data is readily available from the model runs.

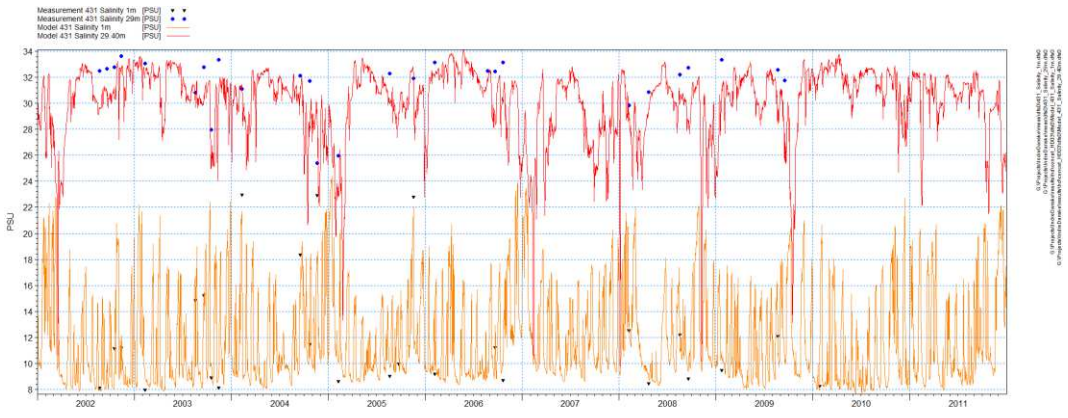

Figure 35: Measured surface (black dots) and bottom (blue dots) salinity compared to modelled salinity at surface (orange line) and at the bottom (red lines), respectively, at the monitoring station Ven (431).

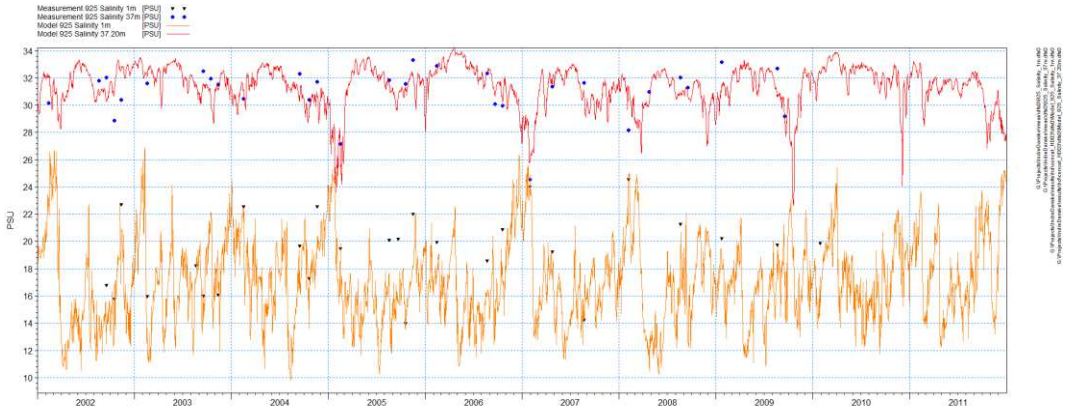

Figure 36: Measured surface (black dots) and bottom (blue dots) salinity concentrations compared to modelled salinity at surface (orange line) and at the bottom (red lines) at the monitoring station at Gniben (925).

Figure 37: Measured surface (black dots) and bottom (blue dots) water temperature compared to modelled temperature at surface (orange line) and at the bottom (red lines) at the monitoring station Ven (431).

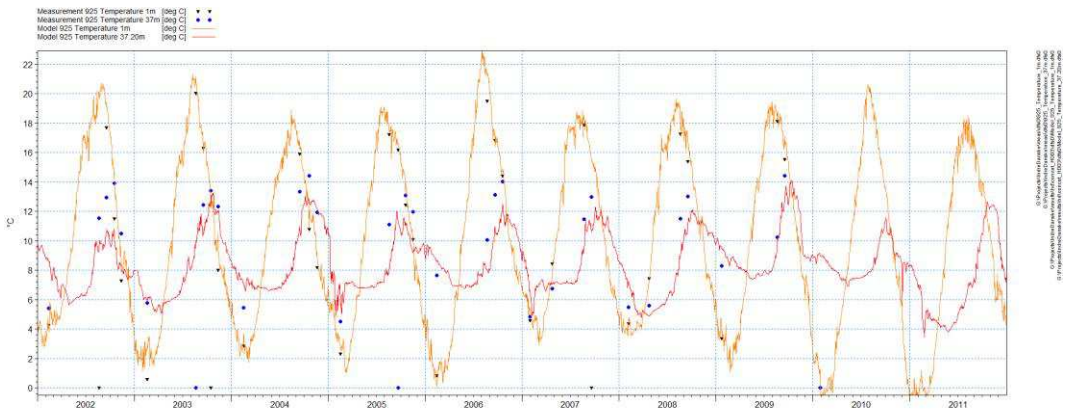

Figure 38: Measured surface (black dots) and bottom (blue dots) water temperature compared to modelled temperature at surface (orange line) and at the bottom (red lines) at the monitoring station Gniben (925).

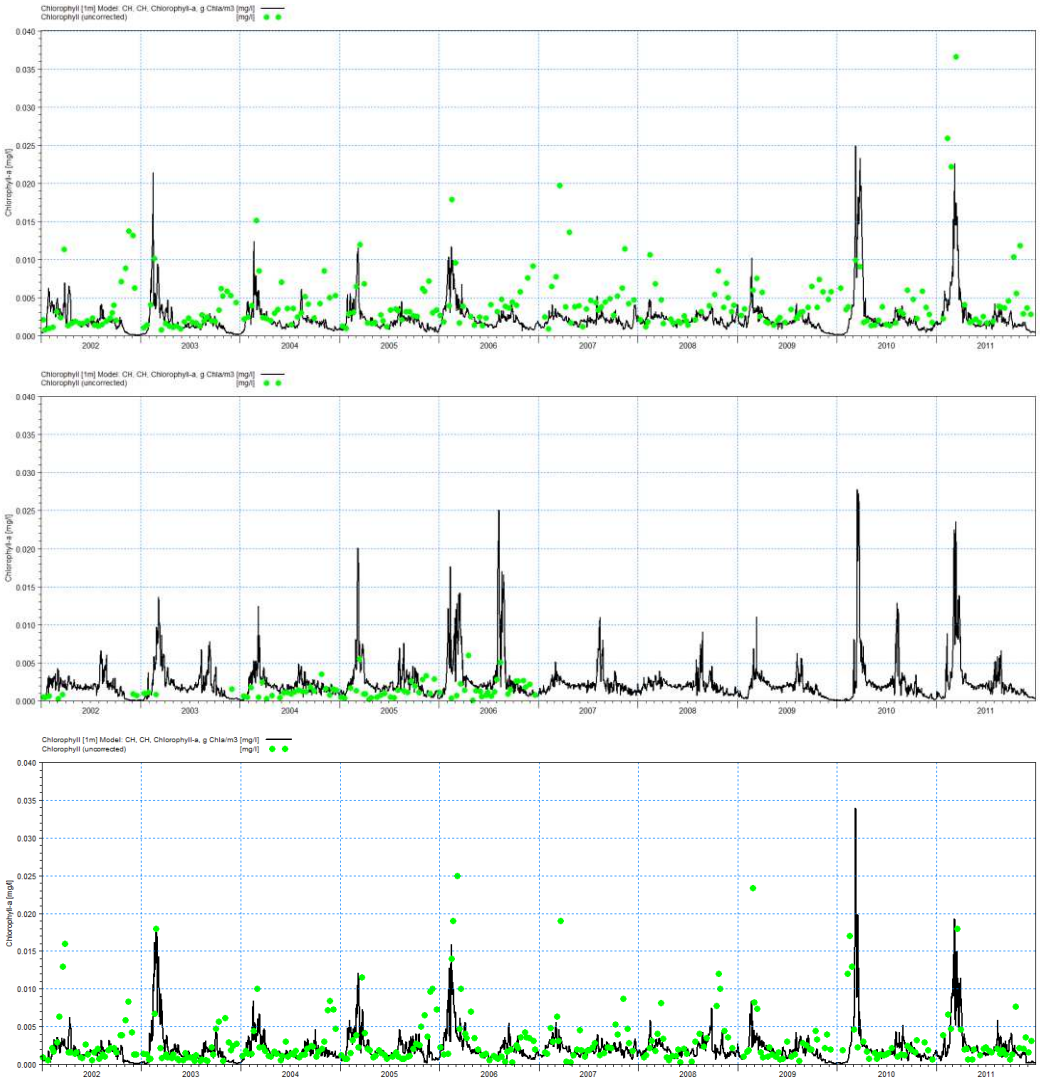

Figure 39: Measurements of surface chlorophyll-a concentrations (green dots) and modelled concentrations (black line). Top panel is from south of Funen, middle panel is from the Sound and bottom panel is from Aarhus Bay.

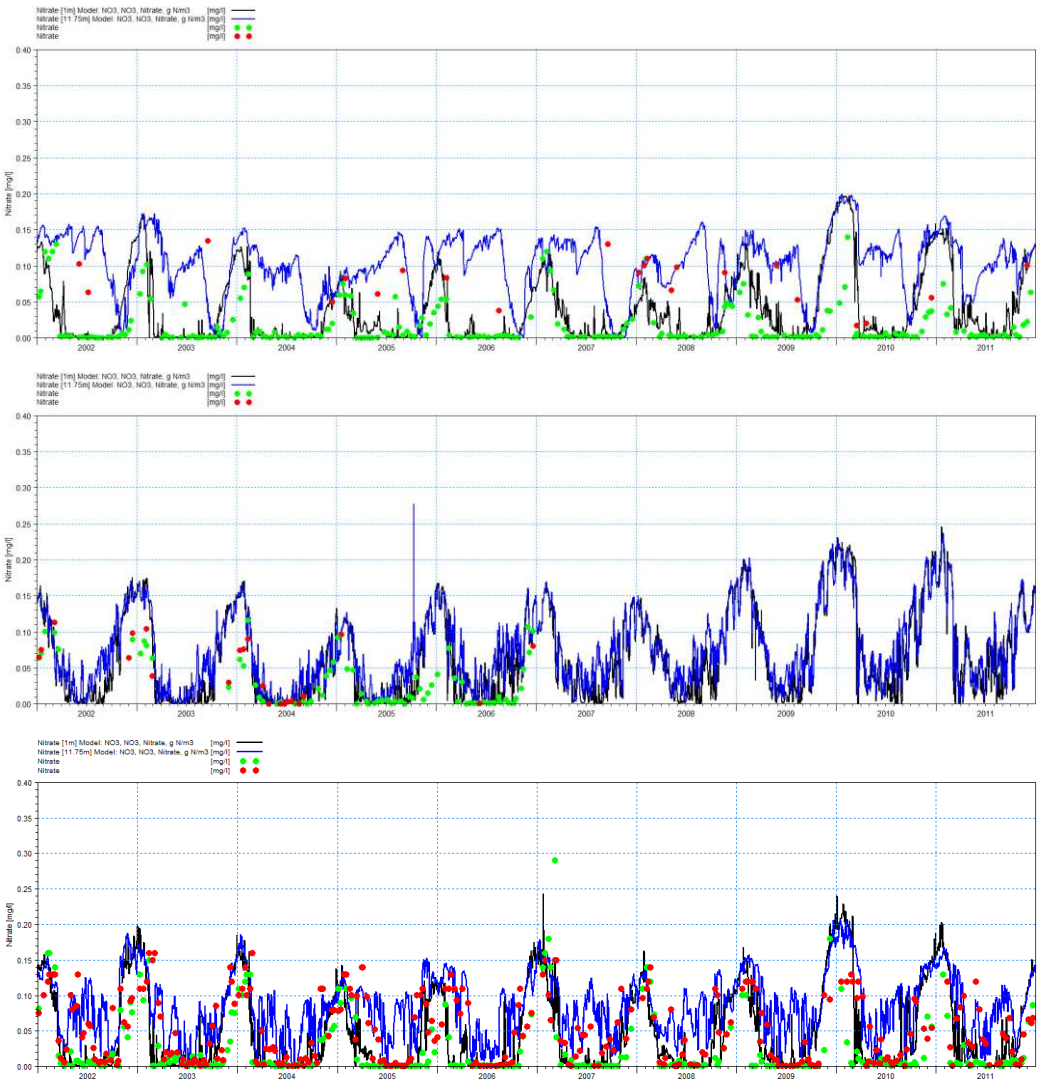

Figure 40: Measurements of surface nitrate concentrations (green dots) and modelled concentrations (black line). Red dots indicate measurements at the bottom and blue line indicated modelled concentrations at the bottom. Top panel is from south of Funen, middle panel is from the Sound and bottom panel is from Aarhus Bay.

Figure 41: Measurements of surface phosphorous concentrations (green dots) and modelled concentrations (black line). Red dots indicate measurements at the bottom and blue line indicated modelled concentrations at the bottom. Top panel is from south of Funen, middle panel is from the Sound and bottom panel is from Aarhus Bay.

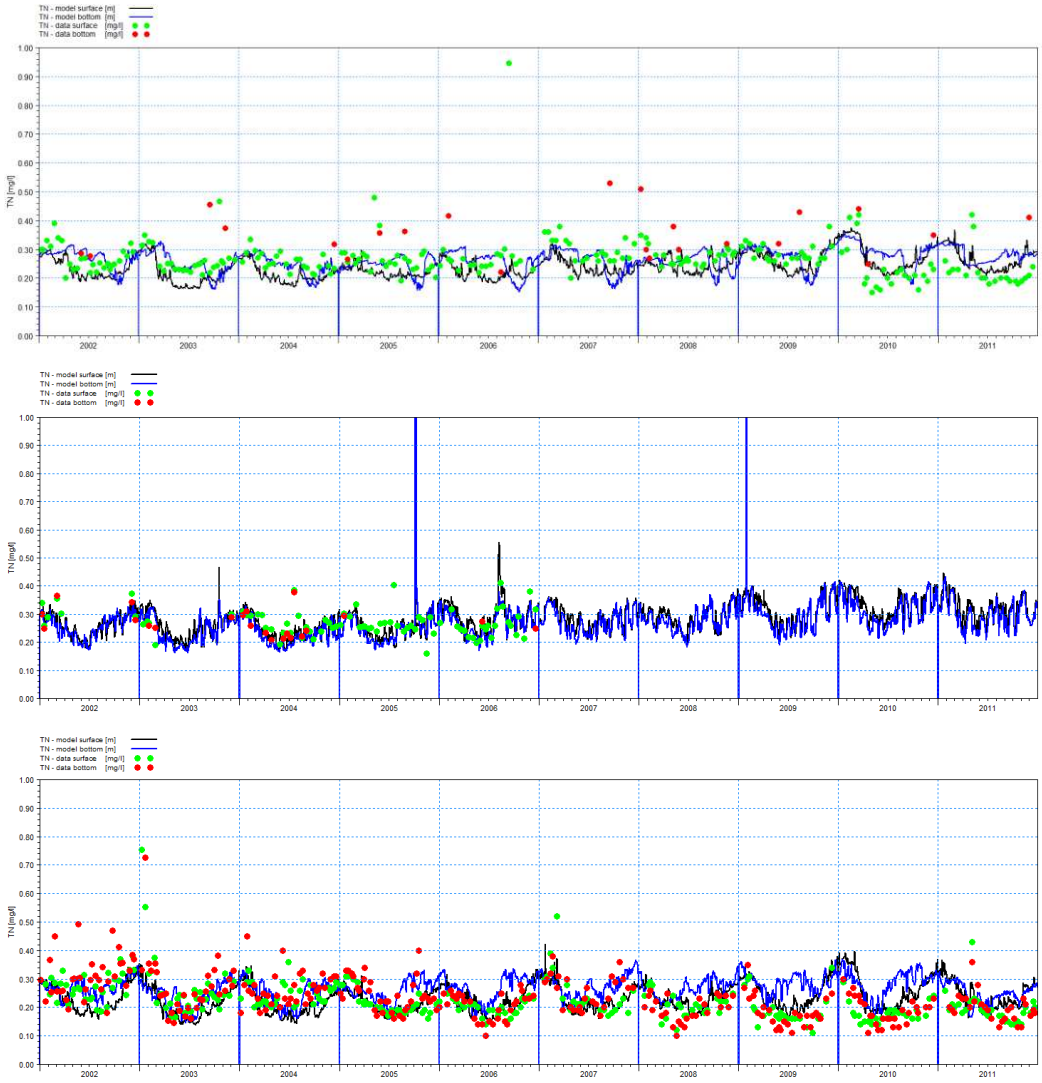

Figure 42: Measurements of surface TN concentrations (green dots) and modelled concentrations (black line). Red dots indicate measurements at the bottom and blue line indicated modelled concentrations at the bottom. Top panel is from south of Funen, middle panel is from the Sound and bottom panel is from Aarhus Bay. The sudden drops at the beginning of each years is an 'artificial' model output due to initialisation, and they are not a result of the modelling.

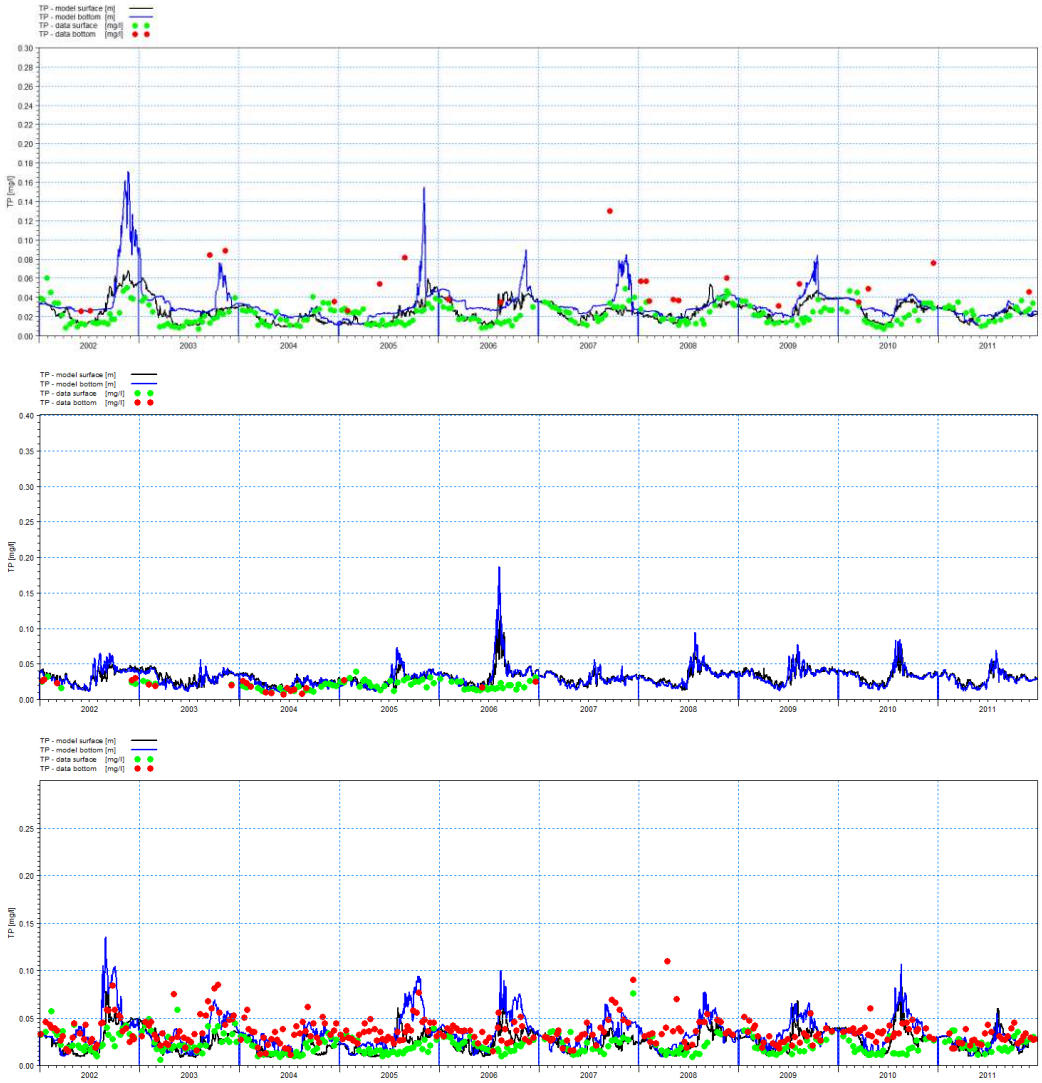

Figure 43: Measurements of surface TP concentrations (green dots) and modelled concentrations (black line). Red dots indicate measurements at the bottom and blue line indicated modelled concentrations at the bottom. Top panel is from south of Funen, middle panel is from the Sound and bottom panel is from Aarhus Bay.

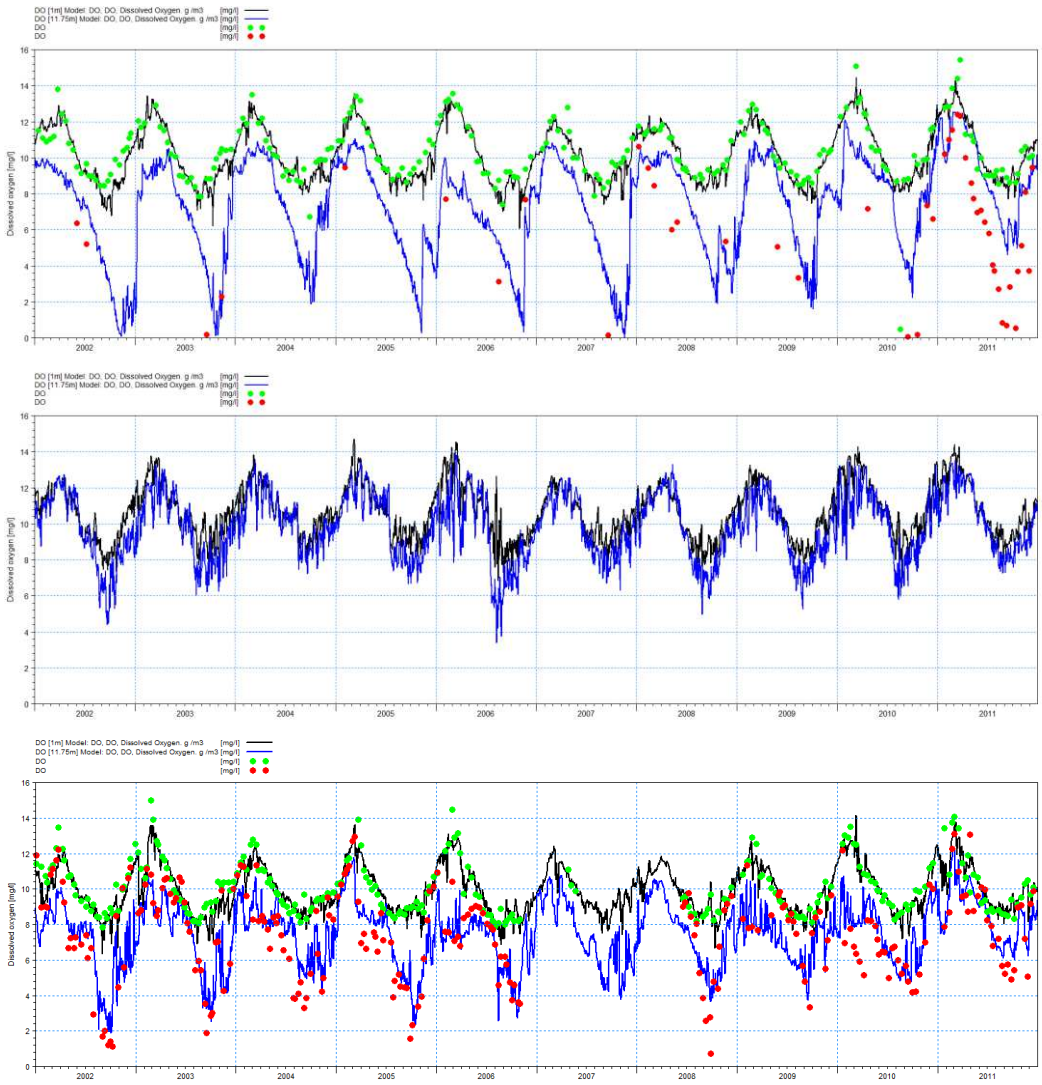

Figure 44: Measurements of surface dissolved oxygen concentrations (green dots) and modelled concentrations (black line). Red dots indicate measurements at the bottom and blue line indicated modelled concentrations at the bottom. Top panel is from south of Funen, middle panel is from the Sound and bottom panel is from Aarhus Bay. No oxygen concentrations exists at the stations in the Sound.

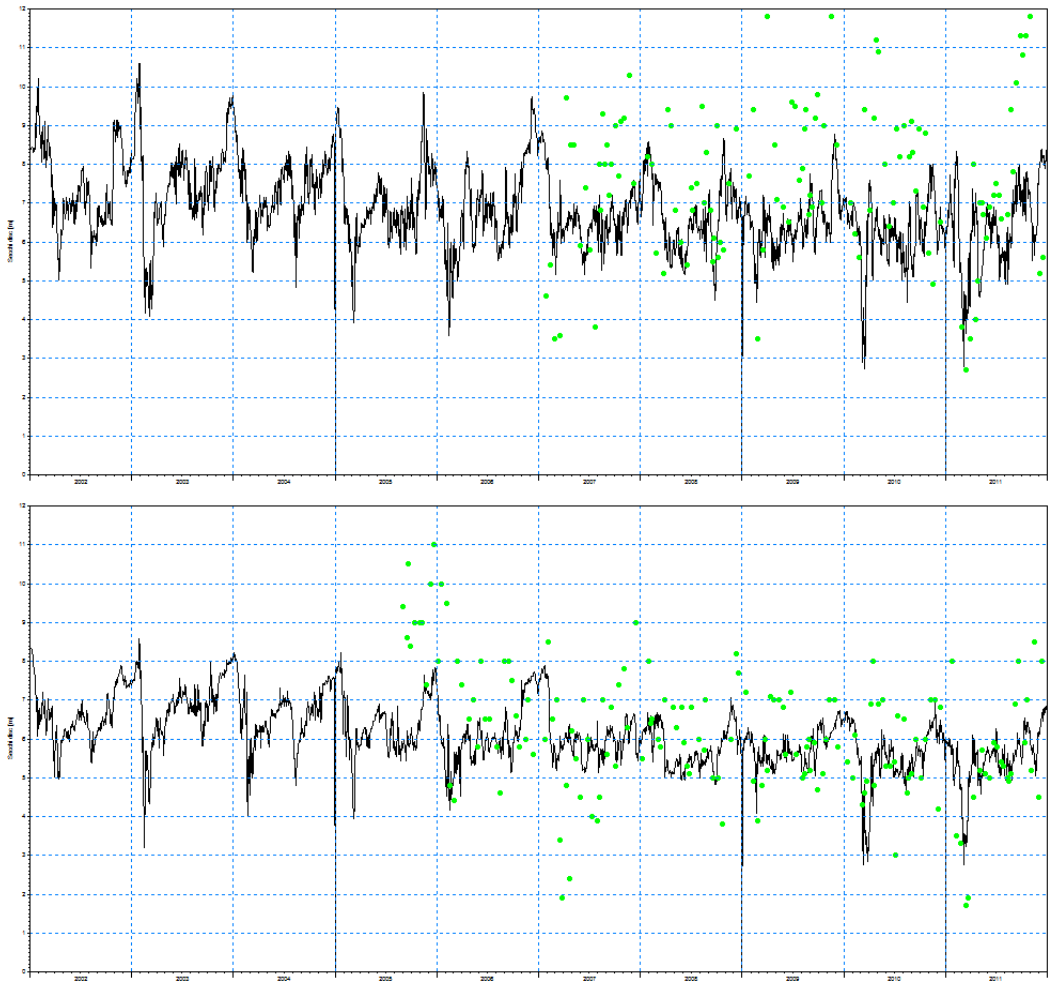

Figure 45: Measurements of Secchi depth (green dots) and modelled Secchi depth (black line). Top panel is from south of Funen and bottom panel is from Aarhus Bay. Data for the Sound station was not available.

MIKE
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MIKE 21 & MIKE 3 Flow Model FM

Hydrodynamic and Transport Module

Scientific Documentation

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CONTENTS

MIKE 21 & MIKE 3 Flow Model FM
Hydrodynamic and Transport Module
Scientific Documentation

1 Introduction

This document presents the scientific background for the new MIKE 21 & MIKE 3 Flow Model FM[1] modelling system developed by DHI Water & Environment. The objective is to provide the user with a detailed description of the flow and transport model equations, numerical discretization and solution methods. Also model validation is discussed in this document.

The MIKE 21 & MIKE 3 Flow Model FM is based on a flexible mesh approach and it has been developed for applications within oceanographic, coastal and estuarine environments. The modelling system may also be applied for studies of overland flooding.

The system is based on the numerical solution of the two/three-dimensional incompressible Reynolds averaged Navier-Stokes equations invoking the assumptions of Boussinesq and of hydrostatic pressure. Thus, the model consists of continuity, momentum, temperature, salinity and density equations and it is closed by a turbulent closure scheme. For the 3D model the free surface is taken into account using a sigma coordinate transformation approach.

The spatial discretization of the primitive equations is performed using a cell-centred finite volume method. The spatial domain is discretized by subdivision of the continuum into non-overlapping elements/cells. In the horizontal plane an unstructured grid is used while in the vertical domain in the 3D model a structured mesh is used. In the 2D model the elements can be triangles or quadrilateral elements. In the 3D model the elements can be prisms or bricks whose horizontal faces are triangles and quadrilateral elements, respectively.

[1] Including the MIKE 21 Flow Model FM (two-dimensional flow) and MIKE 3 Flow Model FM (three-dimensional flow)

2 Governing Equations

2.1 3D Governing Equations in Cartesian Coordinates

2.1.1 Shallow water equations

The model is based on the solution of the three-dimensional incompressible Reynolds averaged Navier-Stokes equations, subject to the assumptions of Boussinesq and of hydrostatic pressure.

The local continuity equation is written as

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=S \tag{2.1}$$

and the two horizontal momentum equations for the x- and y-component, respectively

$$\frac{\partial u}{\partial t}+\frac{\partial u^2}{\partial x}+\frac{\partial vu}{\partial y}+\frac{\partial wu}{\partial z}=fv-g\frac{\partial \eta}{\partial x}-\frac{1}{\rho_0}\frac{\partial p_a}{\partial x}-\frac{g}{\rho_0}\int_z^\eta \frac{\partial \rho}{\partial x}dz-\frac{1}{\rho_0 h}\left(\frac{\partial s_{xx}}{\partial x}+\frac{\partial s_{xy}}{\partial y}\right)+F_u+\frac{\partial}{\partial z}\left(\nu_t\frac{\partial u}{\partial z}\right)+u_s S \tag{2.2}$$

$$\frac{\partial v}{\partial t}+\frac{\partial v^2}{\partial y}+\frac{\partial uv}{\partial x}+\frac{\partial wv}{\partial z}=-fu-g\frac{\partial \eta}{\partial y}-\frac{1}{\rho_0}\frac{\partial p_a}{\partial y}-\frac{g}{\rho_0}\int_z^\eta \frac{\partial \rho}{\partial y}dz-\frac{1}{\rho_0 h}\left(\frac{\partial s_{yx}}{\partial x}+\frac{\partial s_{yy}}{\partial y}\right)+F_v+\frac{\partial}{\partial z}\left(\nu_t\frac{\partial v}{\partial z}\right)+v_s S \tag{2.3}$$

where t is the time; x, y and z are the Cartesian coordinates; η is the surface elevation; d is the still water depth; $h=\eta+d$ is the total water depth; u, v and w are the velocity components in the x, y and z direction; $f=2\Omega\sin\phi$ is the Coriolis parameter (Ω is the angular rate of revolution and ϕ the geographic latitude); g is the gravitational acceleration; ρ is the density of water; s_{xx}, s_{xy}, s_{yx} and s_{yy} are components of the radiation stress tensor; ν_t is the vertical turbulent (or eddy) viscosity; p_a is the atmospheric pressure; ρ_0 is the reference density of water. S is the magnitude of the discharge due to point sources and (u_s, v_s) is the velocity by which the water is discharged into the ambient water. The horizontal stress terms are described using a gradient-stress relation, which is simplified to

$$F_u=\frac{\partial}{\partial x}\left(2A\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(A\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right) \tag{2.4}$$

$$F_v = \frac{\partial}{\partial x}\left(A\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right) + \frac{\partial}{\partial y}\left(2A\frac{\partial v}{\partial y}\right) \tag{2.5}$$

where *A* is the horizontal eddy viscosity.

The surface and bottom boundary condition for *u*, *v* and *w* are

At $z = \eta$:

$$\frac{\partial \eta}{\partial t} + u\frac{\partial \eta}{\partial x} + v\frac{\partial \eta}{\partial y} - w = 0, \quad \left(\frac{\partial u}{\partial z}, \frac{\partial v}{\partial z}\right) = \frac{1}{\rho_0 \nu_t}\left(\tau_{sx}, \tau_{sy}\right) \tag{2.6}$$

At $z = -d$:

$$u\frac{\partial d}{\partial x} + v\frac{\partial d}{\partial y} + w = 0, \quad \left(\frac{\partial u}{\partial z}, \frac{\partial v}{\partial z}\right) = \frac{1}{\rho_0 \nu_t}\left(\tau_{bx}, \tau_{by}\right) \tag{2.7}$$

where $\left(\tau_{sx}, \tau_{sy}\right)$ and $\left(\tau_{bx}, \tau_{by}\right)$ are the *x* and *y* components of the surface wind and bottom stresses.

The total water depth, *h*, can be obtained from the kinematic boundary condition at the surface, once the velocity field is known from the momentum and continuity equations. However, a more robust equation is obtained by vertical integration of the local continuity equation

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} + \frac{\partial h\bar{v}}{\partial y} = hS + \hat{P} - \hat{E} \tag{2.8}$$

where $\hat{P}$ and $\hat{E}$ are precipitation and evaporation rates, respectively, and $\bar{u}$ and $\bar{v}$ are the depth-averaged velocities

$$h\bar{u} = \int_{-d}^{\eta} u\,dz, \quad h\bar{v} = \int_{-d}^{\eta} v\,dz \tag{2.9}$$

The fluid is assumed to be incompressible. Hence, the density, ρ, does not depend on the pressure, but only on the temperature, *T*, and the salinity, *s*, via the equation of state

$$\rho = \rho(T, s) \tag{2.10}$$

Here the UNESCO equation of state is used (see UNESCO, 1981).

2.1.2 Transport equations for salt and temperature

The transports of temperature, *T*, and salinity, *s*, follow the general transport-diffusion equations as

$$\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}+\frac{\partial wT}{\partial z}=F_T+\frac{\partial}{\partial z}\left(D_v\frac{\partial T}{\partial z}\right)+\hat{H}+T_s S \tag{2.11}$$

$$\frac{\partial s}{\partial t}+\frac{\partial us}{\partial x}+\frac{\partial vs}{\partial y}+\frac{\partial ws}{\partial z}=F_s+\frac{\partial}{\partial z}\left(D_v\frac{\partial s}{\partial z}\right)+s_s S \tag{2.12}$$

where D_v is the vertical turbulent (eddy) diffusion coefficient. $\hat{H}$ is a source term due to heat exchange with the atmosphere. T_s and s_s are the temperature and the salinity of the source. *F* are the horizontal diffusion terms defined by

$$(F_T, F_s)=\left[\frac{\partial}{\partial x}\left(D_h\frac{\partial}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_h\frac{\partial}{\partial y}\right)\right](T,s) \tag{2.13}$$

where D_h is the horizontal diffusion coefficient. The diffusion coefficients can be related to the eddy viscosity

$$D_h=\frac{A}{\sigma_T}\quad\text{and}\quad D_v=\frac{\nu_t}{\sigma_T} \tag{2.14}$$

where σ_T is the Prandtl number. In many applications a constant Prandtl number can be used (see Rodi (1984)).

The surface and bottom boundary conditions for the temperature are

At $z=\eta$:

$$D_h\frac{\partial T}{\partial z}=\frac{Q_n}{\rho_0 c_p}+T_p\hat{P}-T_e\hat{E} \tag{2.15}$$

At $z=-d$:

$$\frac{\partial T}{\partial z}=0 \tag{2.16}$$

where Q_n is the surface net heat flux and $c_p=4217\ \mathrm{J/(kg\cdot°K)}$ is the specific heat of the water. A detailed description for determination of $\hat{H}$ and Q_n is given in Section 2.10.

The surface and bottom boundary conditions for the salinity are

At $z = \eta$:

$$\frac{\partial s}{\partial z} = 0 \tag{2.17}$$

At $z = -d$:

$$\frac{\partial s}{\partial z} = 0 \tag{2.18}$$

When heat exchange from the atmosphere is included, the evaporation is defined as

$$\hat{E} = \begin{cases} \dfrac{q_v}{\rho_0 l_v} & q_v > 0 \\ 0 & q_v \le 0 \end{cases} \tag{2.19}$$

where q_v is the latent heat flux and $l_v = 2.5 \cdot 10^6$ is the latent heat of vaporisation of water.

2.1.3 Transport equation for a scalar quantity

The conservation equation for a scalar quantity is given by

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial wC}{\partial z} = F_C + \frac{\partial}{\partial z}\left(D_v \frac{\partial C}{\partial z} \right) - k_p C + C_s S \tag{2.20}$$

where *C* is the concentration of the scalar quantity, k_p is the linear decay rate of the scalar quantity, C_s is the concentration of the scalar quantity at the source and D_v is the vertical diffusion coefficient. F_C is the horizontal diffusion term defined by

$$F_C = \left[\frac{\partial}{\partial x}\left(D_h \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y}\left(D_h \frac{\partial}{\partial y} \right) \right] C \tag{2.21}$$

where D_h is the horizontal diffusion coefficient.

2.1.4 Turbulence model

The turbulence is modelled using an eddy viscosity concept. The eddy viscosity is often described separately for the vertical and the horizontal transport. Here several turbulence models can be applied: a constant viscosity, a vertically parabolic viscosity and a standard k-ε model (Rodi, 1984). In many numerical simulations the small-scale turbulence cannot be resolved with the chosen spatial resolution. This kind of turbulence can be approximated using sub-grid scale models.

Vertical eddy viscosity

The eddy viscosity derived from the log-law is calculated by

$$\nu_t = U_\tau h\left(c_1\frac{z+d}{h}+c_2\left(\frac{z+d}{h}\right)^2\right) \tag{2.22}$$

where $U_\tau = \max(U_{\tau s}, U_{\tau b})$ and c_1 and c_2 are two constants. $U_{\tau s}$ and $U_{\tau b}$ are the friction velocities associated with the surface and bottom stresses, $c_1 = 0.41$ and $c_2 = -0.41$ give the standard parabolic profile.

In applications with stratification the effects of buoyancy can be included explicitly. This is done through the introduction of a Richardson number dependent damping of the eddy viscosity coefficient, when a stable stratification occurs. The damping is a generalisation of the Munk-Anderson formulation (Munk and Anderson, 1948)

$$\nu_t = \nu_t^*(1+aRi)^{-b} \tag{2.23}$$

where ν_t^* is the undamped eddy viscosity and *Ri* is the local gradient Richardson number

$$Ri = -\frac{g}{\rho_0}\frac{\partial\rho}{\partial z}\left(\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial v}{\partial z}\right)^2\right)^{-1} \tag{2.24}$$

$a = 10$ and $b = 0.5$ are empirical constants.

In the k-ε model the eddy-viscosity is derived from turbulence parameters *k* and ε as

$$\nu_t = c_\mu\frac{k^2}{\varepsilon} \tag{2.25}$$

where *k* is the turbulent kinetic energy per unit mass (TKE), ε is the dissipation of TKE and c_μ is an empirical constant.

The turbulent kinetic energy, *k,* and the dissipation of TKE, ε, are obtained from the following transport equations

$$\frac{\partial k}{\partial t}+\frac{\partial uk}{\partial x}+\frac{\partial vk}{\partial y}+\frac{\partial wk}{\partial z} = F_k+\frac{\partial}{\partial z}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial z}\right)+P+B-\varepsilon \tag{2.26}$$

$$\frac{\partial\varepsilon}{\partial t}+\frac{\partial u\varepsilon}{\partial x}+\frac{\partial v\varepsilon}{\partial y}+\frac{\partial w\varepsilon}{\partial z} = F_\varepsilon+\frac{\partial}{\partial z}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial z}\right)+\frac{\varepsilon}{k}\left(c_{1\varepsilon}P+c_{3\varepsilon}B-c_{2\varepsilon}\varepsilon\right) \tag{2.27}$$

where the shear production, *P*, and the buoyancy production, *B*, are given as

$$P = \frac{\tau_{xz}}{\rho_0}\frac{\partial u}{\partial z} + \frac{\tau_{yz}}{\rho_0}\frac{\partial v}{\partial z} \approx \nu_t\left(\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2\right) \tag{2.28}$$

$$B = -\frac{\nu_t}{\sigma_t}N^2 \tag{2.29}$$

with the Brunt-Väisälä frequency, *N*, defined by

$$N^2 = -\frac{g}{\rho_0}\frac{\partial \rho}{\partial z} \tag{2.30}$$

σ_t is the turbulent Prandtl number and σ_k, σ_ε, $c_{1\varepsilon}$, $c_{2\varepsilon}$ and $c_{3\varepsilon}$ are empirical constants. *F* are the horizontal diffusion terms defined by

$$(F_k, F_\varepsilon) = \left[\frac{\partial}{\partial x}\left(D_h\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_h\frac{\partial}{\partial y}\right)\right](k, \varepsilon) \tag{2.31}$$

The horizontal diffusion coefficients are given by $D_h = A/\sigma_k$ and $D_h = A/\sigma_\varepsilon$, respectively.

Several carefully calibrated empirical coefficients enter the k-e turbulence model. The empirical constants are listed in (2.47) (see Rodi, 1984).

Table 2.1 Empirical constants in the k-ε model.

c_μ	$c_{1\varepsilon}$	$c_{2\varepsilon}$	$c_{3\varepsilon}$	σ_t	σ_k	σ_ε
0.09	1.44	1.92	0	0.9	1.0	1.3

At the surface the boundary conditions for the turbulent kinetic energy and its rate of dissipation depend on the wind shear, $U_{\tau s}$

At $z = \eta$:

$$k = \frac{1}{\sqrt{c_\mu}}U_{\tau s}^2 \tag{2.32}$$

$$\varepsilon = \frac{U_{\tau s}^3}{\kappa \Delta z_b} \qquad \text{for} \quad U_{\tau s} > 0$$

$$\frac{\partial k}{\partial z} = 0 \qquad \varepsilon = \frac{\left(k\sqrt{c_\mu}\right)^{3/2}}{a\kappa h} \qquad \text{for} \quad U_{\tau s} = 0 \tag{2.33}$$

where κ=0.4 is the von Kármán constant, $a = 0.07$ is and empirical constant and Δz_s is the distance from the surface where the boundary condition is imposed. At the seabed the boundary conditions are

At $z = -d$:

$$k = \frac{1}{\sqrt{c_\mu}} U_{\tau b}^2 \qquad \varepsilon = \frac{U_{\tau b}^3}{\kappa \Delta z_b} \tag{2.34}$$

where Δz_b is the distance from the bottom where the boundary condition is imposed.

Horizontal eddy viscosity

In many applications a constant eddy viscosity can be used for the horizontal eddy viscosity. Alternatively, Smagorinsky (1963) proposed to express sub-grid scale transports by an effective eddy viscosity related to a characteristic length scale. The subgrid scale eddy viscosity is given by

$$A = c_s^2 l^2 \sqrt{2 S_{ij} S_{ij}} \tag{2.35}$$

where c_s is a constant, l is a characteristic length and the deformation rate is given by

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (i, j = 1,2) \tag{2.36}$$

2.1.5 Governing equations in Cartesian and sigma coordinates

The equations are solved using a vertical σ-transformation

$$\sigma = \frac{z - z_b}{h}, \quad x' = x, \quad y' = y \tag{2.37}$$

where σ varies between 0 at the bottom and 1 at the surface. The coordinate transformation implies relations such as

$$\frac{\partial}{\partial z} = \frac{1}{h}\frac{\partial}{\partial \sigma} \tag{2.38}$$

$$\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) = \left(\frac{\partial}{\partial x'} - \frac{1}{h}\left(-\frac{\partial d}{\partial x} + \sigma \frac{\partial h}{\partial x} \right) \frac{\partial}{\partial \sigma}, \frac{\partial}{\partial y'} - \frac{1}{h}\left(-\frac{\partial d}{\partial y} + \sigma \frac{\partial h}{\partial y} \right) \frac{\partial}{\partial \sigma} \right) \tag{2.39}$$

In this new coordinate system the governing equations are given as

$$\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x'} + \frac{\partial hv}{\partial y'} + \frac{\partial h\omega}{\partial \sigma} = hS \tag{2.40}$$

$$\frac{\partial hu}{\partial t}+\frac{\partial hu^2}{\partial x'}+\frac{\partial hvu}{\partial y'}+\frac{\partial h\omega u}{\partial \sigma}=fvh-gh\frac{\partial \eta}{\partial x'}-\frac{h}{\rho_0}\frac{\partial p_a}{\partial x'}-\frac{hg}{\rho_0}\int_z^\eta \frac{\partial \rho}{\partial x}dz-\frac{1}{\rho_0}\left(\frac{\partial s_{xx}}{\partial x}+\frac{\partial s_{xy}}{\partial y}\right)+hF_u+\frac{\partial}{\partial \sigma}\left(\frac{\nu_v}{h}\frac{\partial u}{\partial \sigma}\right)+hu_sS \quad (2.41)$$

$$\frac{\partial hv}{\partial t}+\frac{\partial huv}{\partial x'}+\frac{\partial hv^2}{\partial y'}+\frac{\partial h\omega v}{\partial \sigma}=-fuh-gh\frac{\partial \eta}{\partial y'}-\frac{h}{\rho_0}\frac{\partial p_a}{\partial y'}-\frac{hg}{\rho_0}\int_z^\eta \frac{\partial \rho}{\partial y}dz-\frac{1}{\rho_0}\left(\frac{\partial s_{yx}}{\partial x}+\frac{\partial s_{yy}}{\partial y}\right)+hF_v+\frac{\partial}{\partial \sigma}\left(\frac{\nu_v}{h}\frac{\partial v}{\partial \sigma}\right)+hv_sS \quad (2.42)$$

$$\frac{\partial hT}{\partial t}+\frac{\partial huT}{\partial x'}+\frac{\partial hvT}{\partial y'}+\frac{\partial h\omega T}{\partial \sigma}=hF_T+\frac{\partial}{\partial \sigma}\left(\frac{D_v}{h}\frac{\partial T}{\partial \sigma}\right)+h\hat{H}+hT_sS \quad (2.43)$$

$$\frac{\partial hs}{\partial t}+\frac{\partial hus}{\partial x'}+\frac{\partial hvs}{\partial y'}+\frac{\partial h\omega s}{\partial \sigma}=hF_s+\frac{\partial}{\partial \sigma}\left(\frac{D_v}{h}\frac{\partial s}{\partial \sigma}\right)+hs_sS \quad (2.44)$$

$$\frac{\partial hk}{\partial t}+\frac{\partial huk}{\partial x'}+\frac{\partial hvk}{\partial y'}+\frac{\partial h\omega k}{\partial \sigma}=hF_k+\frac{1}{h}\frac{\partial}{\partial \sigma}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial \sigma}\right)+h(P+B-\varepsilon) \quad (2.45)$$

$$\frac{\partial h\varepsilon}{\partial t}+\frac{\partial hu\varepsilon}{\partial x'}+\frac{\partial hv\varepsilon}{\partial y'}+\frac{\partial h\omega\varepsilon}{\partial \sigma}=hF_\varepsilon+\frac{1}{h}\frac{\partial}{\partial \sigma}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial \sigma}\right)+h\frac{\varepsilon}{k}\left(c_{1\varepsilon}P+c_{3\varepsilon}B-c_{2\varepsilon}\varepsilon\right) \quad (2.46)$$

$$\frac{\partial hC}{\partial t}+\frac{\partial huC}{\partial x'}+\frac{\partial hvC}{\partial y'}+\frac{\partial h\omega C}{\partial \sigma}=hF_C+\frac{\partial}{\partial \sigma}\left(\frac{D_v}{h}\frac{\partial C}{\partial \sigma}\right)-hk_pC+hC_sS \quad (2.47)$$

The modified vertical velocity is defined by

$$\omega=\frac{1}{h}\left[w+u\frac{\partial d}{\partial x'}+v\frac{\partial d}{\partial y'}-\sigma\left(\frac{\partial h}{\partial t}+u\frac{\partial h}{\partial x'}+v\frac{\partial h}{\partial y'}\right)\right] \quad (2.48)$$

The modified vertical velocity is the velocity across a level of constant σ. The horizontal diffusion terms are defined as

$$hF_u\approx\frac{\partial}{\partial x}\left(2hA\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(hA\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right) \quad (2.49)$$

$$hF_v \approx \frac{\partial}{\partial x}\left(hA\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right)+\frac{\partial}{\partial y}\left(2hA\frac{\partial v}{\partial y}\right) \tag{2.50}$$

$$h(F_T,F_s,F_k,F_\varepsilon,F_c) \approx \left[\frac{\partial}{\partial x}\left(hD_h\frac{\partial}{\partial x}\right)+\frac{\partial}{\partial y}\left(hD_h\frac{\partial}{\partial y}\right)\right](T,s,k,\varepsilon,C) \tag{2.51}$$

The boundary condition at the free surface and at the bottom are given as follows

At σ=1:

$$\omega=0,\quad \left(\frac{\partial u}{\partial \sigma},\frac{\partial v}{\partial \sigma}\right)=\frac{h}{\rho_0\nu_t}\left(\tau_{sx},\tau_{sy}\right) \tag{2.52}$$

At σ=0:

$$\omega=0,\quad \left(\frac{\partial u}{\partial \sigma},\frac{\partial v}{\partial \sigma}\right)=\frac{h}{\rho_0\nu_t}\left(\tau_{bx},\tau_{by}\right) \tag{2.53}$$

The equation for determination of the water depth is not changed by the coordinate transformation. Hence, it is identical to Eq. (2.6).

2.2 3D Governing Equations in Spherical and Sigma Coordinates

In spherical coordinates the independent variables are the longitude, λ , and the latitude, ϕ . The horizontal velocity field (*u,v*) is defined by

$$u = R\cos\phi\frac{d\lambda}{dt} \qquad v = R\frac{d\phi}{dt} \tag{2.54}$$

where *R* is the radius of the earth.

In this coordinate system the governing equations are given as (all superscripts indicating the horizontal coordinate in the new coordinate system are dropped in the following for notational convenience)

$$\frac{\partial h}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial hu}{\partial \lambda}+\frac{\partial hv\cos\phi}{\partial \phi}\right)+\frac{\partial h\omega}{\partial \sigma}=hS \tag{2.55}$$

$$\frac{\partial hu}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial hu^2}{\partial\lambda}+\frac{\partial hvu\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega u}{\partial\sigma}=\left(f+\frac{u}{R}\tan\phi\right)vh-$$
$$\frac{1}{R\cos\phi}\left(gh\frac{\partial\eta}{\partial\lambda}+\frac{1}{\rho_0}\frac{\partial p_a}{\partial\lambda}+\frac{g}{\rho_0}\int_z^\eta\frac{\partial\rho}{\partial\lambda}dz+\frac{1}{\rho_0}\left(\frac{\partial s_{xx}}{\partial\lambda}+\cos\phi\frac{\partial s_{xy}}{\partial\phi}\right)\right)+ \quad (2.56)$$
$$hF_u+\frac{\partial}{\partial\sigma}\left(\frac{\nu_v}{h}\frac{\partial u}{\partial\sigma}\right)+hu_sS$$

$$\frac{\partial hv}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial huv}{\partial\lambda}+\frac{\partial hv^2\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega v}{\partial\sigma}=-\left(f+\frac{u}{R}\tan\phi\right)uh-$$
$$\frac{1}{R}\left(gh\frac{\partial\eta}{\partial\phi}+\frac{1}{\rho_0}\frac{\partial p_a}{\partial\phi}+\frac{g}{\rho_0}\int_z^\eta\frac{\partial\rho}{\partial\phi}dz+\frac{1}{\rho_0}\left(\frac{1}{\cos\phi}\frac{\partial s_{yx}}{\partial\lambda}+\frac{\partial s_{yy}}{\partial\phi}\right)\right)+ \quad (2.57)$$
$$hF_v+\frac{\partial}{\partial\sigma}\left(\frac{\nu_v}{h}\frac{\partial v}{\partial\sigma}\right)+hv_sS$$

$$\frac{\partial hT}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial huT}{\partial\lambda}+\frac{\partial hvT\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega T}{\partial\sigma}= \quad (2.58)$$
$$hF_T+\frac{\partial}{\partial\sigma}\left(\frac{D_v}{h}\frac{\partial T}{\partial\sigma}\right)+h\hat{H}+hT_sS$$

$$\frac{\partial hs}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial hus}{\partial\lambda}+\frac{\partial hvs\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega s}{\partial\sigma}= \quad (2.59)$$
$$hF_s+\frac{\partial}{\partial\sigma}\left(\frac{D_v}{h}\frac{\partial s}{\partial\sigma}\right)+hs_sS$$

$$\frac{\partial hk}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial huk}{\partial\lambda}+\frac{\partial hvk\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega k}{\partial\sigma}= \quad (2.60)$$
$$hF_k+\frac{1}{h}\frac{\partial}{\partial\sigma}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial\sigma}\right)+h(P+B-\varepsilon)$$

$$\frac{\partial h\varepsilon}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial hu\varepsilon}{\partial\lambda}+\frac{\partial hv\varepsilon\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega\varepsilon}{\partial\sigma}= \quad (2.61)$$
$$hF_\varepsilon+\frac{1}{h}\frac{\partial}{\partial\sigma}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial\sigma}\right)+h\frac{\varepsilon}{k}\left(c_{1\varepsilon}P+c_{3\varepsilon}B-c_{2\varepsilon}\varepsilon\right)$$

$$\frac{\partial hC}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial huC}{\partial\lambda}+\frac{\partial hvC\cos\phi}{\partial\phi}\right)+\frac{\partial h\omega C}{\partial\sigma}= \quad (2.62)$$
$$hF_C+\frac{\partial}{\partial\sigma}\left(\frac{D_v}{h}\frac{\partial C}{\partial\sigma}\right)-hk_pC+hC_sS$$

The modified vertical velocity in spherical coordinates is defined by

$$\omega = \frac{1}{h}\left[w + \frac{u}{R\cos\phi}\frac{\partial d}{\partial \lambda} + \frac{v}{R}\frac{\partial d}{\partial y} - \sigma\left(\frac{\partial h}{\partial t} + \frac{u}{R\cos\phi}\frac{\partial h}{\partial \lambda} + \frac{v}{R}\frac{\partial h}{\partial \phi}\right)\right] \tag{2.63}$$

The equation determining the water depth in spherical coordinates is given as

$$\frac{\partial h}{\partial t} + \frac{1}{R\cos\phi}\left(\frac{\partial h\bar{u}}{\partial \lambda} + \frac{\partial h\bar{v}\cos\phi}{\partial \phi}\right) = hS \tag{2.64}$$

2.3 2D Governing Equations in Cartesian Coordinates

2.3.1 Shallow water equations

Integration of the horizontal momentum equations and the continuity equation over depth $h = \eta + d$ the following two-dimensional shallow water equations are obtained

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} + \frac{\partial h\bar{v}}{\partial y} = hS \tag{2.65}$$

$$\begin{aligned}\frac{\partial h\bar{u}}{\partial t} + \frac{\partial h\bar{u}^2}{\partial x} + \frac{\partial h\overline{vu}}{\partial y} = {} & f\bar{v}h - gh\frac{\partial \eta}{\partial x} - \frac{h}{\rho_0}\frac{\partial p_a}{\partial x} - \\ & \frac{gh^2}{2\rho_0}\frac{\partial \rho}{\partial x} + \frac{\tau_{sx}}{\rho_0} - \frac{\tau_{bx}}{\rho_0} - \frac{1}{\rho_0}\left(\frac{\partial s_{xx}}{\partial x} + \frac{\partial s_{xy}}{\partial y}\right) + \\ & \frac{\partial}{\partial x}\left(hT_{xx}\right) + \frac{\partial}{\partial y}\left(hT_{xy}\right) + hu_s S\end{aligned} \tag{2.66}$$

$$\begin{aligned}\frac{\partial h\bar{v}}{\partial t} + \frac{\partial h\overline{uv}}{\partial x} + \frac{\partial h\bar{v}^2}{\partial y} = {} & -f\bar{u}h - gh\frac{\partial \eta}{\partial y} - \frac{h}{\rho_0}\frac{\partial p_a}{\partial y} - \\ & \frac{gh^2}{2\rho_0}\frac{\partial \rho}{\partial y} + \frac{\tau_{sy}}{\rho_0} - \frac{\tau_{by}}{\rho_0} - \frac{1}{\rho_0}\left(\frac{\partial s_{yx}}{\partial x} + \frac{\partial s_{yy}}{\partial y}\right) + \\ & \frac{\partial}{\partial x}\left(hT_{xy}\right) + \frac{\partial}{\partial y}\left(hT_{yy}\right) + hv_s S\end{aligned} \tag{2.67}$$

The overbar indicates a depth average value. For example, $\bar{u}$ and $\bar{v}$ are the depth-averaged velocities defined by

$$h\bar{u} = \int_{-d}^{\eta} u\,dz, \quad h\bar{v} = \int_{-d}^{\eta} v\,dz \tag{2.68}$$

The lateral stresses T_{ij} include viscous friction, turbulent friction and differential advection. They are estimated using an eddy viscosity formulation based on of the depth average velocity gradients

$$T_{xx} = 2A\frac{\partial \bar{u}}{\partial x}, \quad T_{xy} = A\left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x}\right), \quad T_{yy} = 2A\frac{\partial \bar{v}}{\partial y} \tag{2.69}$$

2.3.2 Transport equations for salt and temperature

Integrating the transport equations for salt and temperature over depth the following two-dimensional transport equations are obtained

$$\frac{\partial h\bar{T}}{\partial t} + \frac{\partial h\bar{u}\bar{T}}{\partial x} + \frac{\partial h\bar{v}\bar{T}}{\partial y} = hF_T + h\hat{H} + hT_s S \tag{2.70}$$

$$\frac{\partial h\bar{s}}{\partial t} + \frac{\partial h\bar{u}\bar{s}}{\partial x} + \frac{\partial h\bar{v}\bar{s}}{\partial y} = hF_s + hs_s S \tag{2.71}$$

where $\bar{T}$ and $\bar{s}$ is the depth average temperature and salinity.

2.3.3 Transport equations for a scalar quantity

Integrating the transport equations for a scalar quantity over depth the following two-dimensional transport equations are obtained

$$\frac{\partial h\bar{C}}{\partial t} + \frac{\partial h\bar{u}\bar{C}}{\partial x} + \frac{\partial h\bar{v}\bar{C}}{\partial y} = hF_C - hk_p\bar{C} + hC_s S \tag{2.72}$$

where $\bar{C}$ is the depth average scalar quantity.

2.4 2D Governing Equations in Spherical Coordinates

In spherical coordinates the independent variables are the longitude, λ ,and the latitude, ϕ . The horizontal velocity field (u,v) is defined by

$$\bar{u} = R\cos\phi\frac{d\lambda}{dt} \qquad \bar{v} = R\frac{d\phi}{dt} \tag{2.73}$$

where R is the radius of the earth.

In spherical coordinates the governing equation can be written

$$\frac{\partial h}{\partial t} + \frac{1}{R\cos\phi}\left(\frac{\partial h\bar{u}}{\partial \lambda} + \frac{\partial h\bar{v}\cos\phi}{\partial \phi}\right) = 0 \tag{2.74}$$

$$\frac{\partial h\bar{u}}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial h\bar{u}^2}{\partial\lambda}+\frac{\partial h\overline{vu}\cos\phi}{\partial\phi}\right)=\left(f+\frac{\bar{u}}{R}\tan\phi\right)\bar{v}h$$
$$-\frac{1}{R\cos\phi}\left(gh\frac{\partial\eta}{\partial\lambda}-\frac{h}{\rho_0}\frac{\partial p_a}{\partial\lambda}+\frac{gh^2}{2\rho_0}\frac{\partial\rho}{\partial\lambda}+\frac{1}{\rho_0}\left(\frac{\partial s_{xx}}{\partial\lambda}+\cos\phi\frac{\partial s_{xy}}{\partial\phi}\right)\right)+ \quad (2.75)$$
$$\frac{\tau_{sx}}{\rho_0}-\frac{\tau_{bx}}{\rho_0}+\frac{\partial}{\partial x}\left(hT_{xx}\right)+\frac{\partial}{\partial y}\left(hT_{xy}\right)+hu_sS$$

$$\frac{\partial h\bar{v}}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial h\overline{uv}}{\partial\lambda}+\frac{\partial h\bar{v}^2\cos\varphi}{\partial\iota}\right)=-\left(f+\frac{\bar{u}}{R}\tan\phi\right)\bar{u}h$$
$$-\frac{1}{R}\left(gh\frac{\partial\eta}{\partial\phi}-\frac{h}{\rho_0}\frac{\partial p_a}{\partial\phi}+\frac{gh^2}{2\rho_0}\frac{\partial\rho}{\partial\phi}+\frac{1}{\rho_0}\left(\frac{1}{\cos\phi}\frac{\partial s_{yx}}{\partial\lambda}+\frac{\partial s_{yy}}{\partial\phi}\right)\right)+ \quad (2.76)$$
$$\frac{\tau_{sy}}{\rho_0}-\frac{\tau_{by}}{\rho_0}+\frac{\partial}{\partial x}\left(hT_{xy}\right)+\frac{\partial}{\partial y}\left(hT_{yy}\right)+hv_sS$$

$$\frac{\partial h\bar{T}}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial h\bar{u}\bar{T}}{\partial\lambda}+\frac{\partial h\bar{v}\bar{T}\cos\phi}{\partial\phi}\right)=hF_T+h\hat{H}+hT_sS \quad (2.77)$$

$$\frac{\partial h\bar{s}}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial h\bar{u}\bar{s}}{\partial\lambda}+\frac{\partial h\bar{v}\bar{s}\cos\phi}{\partial\phi}\right)=hF_s+hs_sS \quad (2.78)$$

$$\frac{\partial h\bar{C}}{\partial t}+\frac{1}{R\cos\phi}\left(\frac{\partial h\bar{u}\bar{C}}{\partial\lambda}+\frac{\partial h\bar{v}\bar{C}\cos\phi}{\partial\phi}\right)=hF_C-hk_p\bar{C}+hC_sS \quad (2.79)$$

2.5 Bottom Stress

The bottom stress, $\vec{\tau}_b=(\tau_{bx},\tau_{by})$, is determined by a quadratic friction law

$$\frac{\vec{\tau}_b}{\rho_0}=c_f\vec{u}_b|\vec{u}_b| \quad (2.80)$$

where c_f is the drag coefficient and $\vec{u}_b=(u_b,v_b)$ is the flow velocity above the bottom. The friction velocity associated with the bottom stress is given by

$$U_{\tau b}=\sqrt{c_f|u_b|^2} \quad (2.81)$$

For two-dimensional calculations $\vec{u}_b$ is the depth-average velocity and the drag coefficient can be determined from the Chezy number, C, or the Manning number, M

$$c_f=\frac{g}{C^2} \quad (2.82)$$

$$c_f = \frac{g}{\left(Mh^{1/6}\right)^2} \tag{2.83}$$

For three-dimensional calculations $\vec{u}_b$ is the velocity at a distance Δz_b above the sea bed and the drag coefficient is determined by assuming a logarithmic profile between the seabed and a point Δz_b above the seabed

$$c_f = \frac{1}{\left(\frac{1}{\kappa}\ln\left(\frac{\Delta z_b}{z_0}\right)\right)^2} \tag{2.84}$$

where κ=0.4 is the von Kármán constant and z_0 is the bed roughness length scale. When the boundary surface is rough, z_0, depends on the roughness height, k_s

$$z_0 = mk_s \tag{2.85}$$

where m is approximately 1/30.

Note, that the Manning number can be estimated from the bed roughness length using the following

$$M = \frac{25.4}{k_s^{1/6}} \tag{2.86}$$

The wave induced bed resistance can be determined from

$$c_f = \left(\frac{u_{fc}}{u_b}\right)^2 \tag{2.87}$$

where U_{fc} is the friction velocity calculated by considering the conditions in the wave boundary layer. For a detailed description of the wave induced bed resistance, see Fredsøe (1984) and Jones et.al. (2014).

2.6 Wind Stress

In areas not covered by ice the surface stress, $\vec{\tau}_s = (\tau_{sx}, \tau_{sy})$, is determined by the winds above the surface. The stress is given by the following empirical relation

$$\bar{\tau}_s = \rho_a c_d |u_w| \bar{u}_w \tag{2.88}$$

where ρ_a is the density of air, c_d is the drag coefficient of air, and $\vec{u}_w = (u_w, v_w)$ is the wind speed 10 m above the sea surface. The friction velocity associated with the surface stress is given by

$$U_{\tau s} = \sqrt{\frac{\rho_a c_f \left|\bar{u}_w\right|^2}{\rho_0}} \tag{2.89}$$

The drag coefficient can either be a constant value or depend on the wind speed. The empirical formula proposed by Wu (1980, 1994) is used for the parameterisation of the drag coefficient.

$$c_f = \begin{cases} c_a & w_{10} < w_a \\ c_a + \dfrac{c_b - c_a}{w_b - w_a}\left(w_{10} - w_a\right) & w_a \le w_{10} < w_b \\ c_b & w_{10} \ge w_b \end{cases} \tag{2.90}$$

where c_a, c_b, w_a and w_b are empirical factors and w_{10} is the wind velocity 10 m above the sea surface. The default values for the empirical factors are $c_a = 1.255 \cdot 10^{-3}$, $c_b = 2.425 \cdot 10^{-3}$, $w_a = 7$ m/s and $w_b = 25$ m/s. These give generally good results for open sea applications. Field measurements of the drag coefficient collected over lakes indicate that the drag coefficient is larger than open ocean data. For a detailed description of the drag coefficient see Geernaert and Plant (1990).

2.7 Ice Coverage

It is possible to take into account the effects of ice coverage on the flow field.

In areas where the sea is covered by ice the wind stress is excluded. Instead, the surface stress is caused by the ice roughness. The surface stress, $\vec{\tau}_s = (\tau_{sx}, \tau_{sy})$, is determined by a quadratic friction law

$$\frac{\vec{\tau}_s}{\rho_0} = c_f \vec{u}_s \left|\vec{u}_s\right| \tag{2.91}$$

where c_f is the drag coefficient and $\vec{u}_s = (u_s, v_s)$ is the flow velocity below the surface. The friction velocity associated with the surface stress is given by

$$U_{\tau s} = \sqrt{c_f \left|u_s\right|^2} \tag{2.92}$$

For two-dimensional calculations $\vec{u}_s$ is the depth-average velocity and the drag coefficient can be determined from the Manning number, M

$$c_f = \frac{g}{\left(M h^{1/6}\right)^2} \tag{2.93}$$

The Manning number is estimated from the bed roughness length using the following

$$M = \frac{25.4}{k_s^{1/6}} \tag{2.94}$$

For three-dimensional calculations $\vec{u}_s$ is the velocity at a distance Δz_s below the surface and the drag coefficient is determined by assuming a logarithmic profile between the surface and a point Δz_b below the surface

$$c_f = \frac{1}{\left(\frac{1}{\kappa}\ln\left(\frac{\Delta z_s}{z_0}\right)\right)^2} \tag{2.95}$$

where κ=0.4 is the von Kármán constant and z_0 is the bed roughness length scale. When the boundary surface is rough, z_0, depends on the roughness height, k_s

$$z_0 = mk_s \tag{2.96}$$

where m is approximately 1/30.

2.8 Tidal Potential

The tidal potential is a force, generated by the variations in gravity due to the relative motion of the earth, the moon and the sun that act throughout the computational domain. The forcing is expanded in frequency space and the potential considered as the sum of a number of terms each representing different tidal constituents. The forcing is implemented as a so-called equilibrium tide, which can be seen as the elevation that theoretically would occur, provided the earth was covered with water. The forcing enters the momentum equations (e.g. (2.66) or (2.75)) as an additional term representing the gradient of the equilibrium tidal elevations, such that the elevation η can be seen as the sum of the actual elevation and the equilibrium tidal potential.

$$\eta = \eta_{ACTUAL} + \eta_T \tag{2.97}$$

The equilibrium tidal potential η_T is given as

$$\eta_T = \sum_i e_i H_i f_i L_i \cos(2\pi \frac{t}{T_i} + b_i + i_0 x) \tag{2.98}$$

where η_T is the equilibrium tidal potential, *i* refers to constituent number (note that the constituents here are numbered sequentially), e_i is a correction for earth tides based on Love numbers, H_i is the amplitude, f_i is a nodal factor, L_i is given below, *t* is time, T_i is the period of the constituent, b_i is the phase and *x* is the longitude of the actual position.

The phase *b* is based on the motion of the moon and the sun relative to the earth and can be given by

$$b_i = (i_1 - i_0)s + (i_2 + i_0)h + i_3 p + i_4 N + i_5 p_s + u_i \sin(N) \tag{2.99}$$

where i_0 is the species, i_1 to i_5 are Doodson numbers, u is a nodal modulation factor (see Table 2.3) and the astronomical arguments s, h, p, N and p_s are given in Table 2.2.

Table 2.2 Astronomical arguments (Pugh, 1987)

Mean longitude of the moon	s	$277.02+481267.89T+0.0011T^2$
Mean longitude of the sun	h	$280.19+36000.77T+0.0003T^2$
Longitude of lunar perigee	p	$334.39+4069.04T-0.0103T^2$
Longitude of lunar ascending node	N	$259.16-1934.14T+0.0021T^2$
Longitude of perihelion	p_s	$281.22+1.72T+0.0005T^2$

In Table 2.2 the time, T, is in Julian century from January 1 1900 UTC, thus T = (365(y – 1900) + (d – 1) + i)/36525 and i = *int* (y-1901)/4), y is year and d is day number

L depends on species number i_0 and latitude y as

$i_0 = 0$ $\quad L = 3\sin^2(y) - 1$

$i_0 = 1$ $\quad L = \sin(2y)$

$i_0 = 2$ $\quad L = \cos^2(y)$

The nodal factor f_i represents modulations to the harmonic analysis and can for some constituents be given as shown in Table 2.3.

Table 2.3 Nodal modulation terms (Pugh, 1987)

	f_i	u_i
M_m	1.000 - 0.130 cos(N)	0
M_f	1.043 + 0.414 cos(N)	-23.7 sin(N)
Q_1, O_1	1.009 + 0.187 cos(N)	10.8 sin(N)
K_1	1.006 + 0.115 cos(N)	-8.9 sin(N)
$2N_2$, μ_2, ν_2, N_2, M_2	1.000 - 0.037 cos(N)	-2.1 sin(N)
K_2	1.024 + 0.286 cos(N)	-17.7 sin(N)

2.9 Wave Radiation

The second order stresses due to breaking of short period waves can be included in the simulation. The radiation stresses act as driving forces for the mean flow and can be used to calculate wave induced flow. For 3D simulations a simple approach is used. Here a uniform variation is used for the vertical variation in radiation stress.

2.10 Heat Exchange

The heat exchange with the atmosphere is calculated on basis of the four physical processes

- Latent heat flux (or the heat loss due to vaporisation)
- Sensible heat flux (or the heat flux due to convection)
- Net short wave radiation
- Net long wave radiation

Latent and sensible heat fluxes and long-wave radiation are assumed to occur at the surface. The absorption profile for the short-wave flux is approximated using Beer's law. The attenuation of the light intensity is described through the modified Beer's law as

$$I(d) = (1-\beta) I_0 e^{-\lambda d} \tag{2.100}$$

where $I(d)$ is the intensity at depth *d* below the surface; I_0 is the intensity just below the water surface; β is a quantity that takes into account that a fraction of light energy (the infrared) is absorbed near the surface; λ is the light extinction coefficient. Typical values for β and λ are 0.2-0.6 and 0.5-1.4 m^{-1}, respectively. β and λ are user-specified constants. The default values are $\beta = 0.3$ and $\lambda = 1.0\ m^{-1}$. The fraction of the light energy that is absorbed near the surface is βI_0. The net short-wave radiation, $q_{sr,net}$, is attenuated as described by the modified Beer's law. Hence the surface net heat flux is given by

$$Q_n = q_v + q_c + \beta q_{sr,net} + q_{lr,net} \tag{2.101}$$

For three-dimensional calculations the source term $\hat{H}$ is given by

$$\hat{H} = \frac{\partial}{\partial z}\left(\frac{q_{sr,net}(1-\beta) e^{-\lambda(\eta - z)}}{\rho_0 c_p} \right) = \frac{q_{sr,net}(1-\beta)\dfrac{e^{-\lambda(\eta-z)}}{\lambda}}{\rho_0 c_p} \tag{2.102}$$

For two-dimensional calculations the source term $\hat{H}$ is given by

$$\hat{H} = \frac{q_v + q_c + q_{sr,net} + q_{lr,net}}{\rho_0 c_p} \tag{2.103}$$

The calculation of the latent heat flux, sensible heat flux, net short wave radiation, and net long wave radiation as described in the following sections.

In areas covered by ice the heat exchange is excluded.

2.10.1 Vaporisation

Dalton's law yields the following relationship for the vaporative heat loss (or latent flux), see Sahlberg, 1984

$$q_v = LC_e(a_1 + b_1 W_{2m})(Q_{water} - Q_{air}) \tag{2.104}$$

where $L = 2.5 \cdot 10^6$ J / kg is the latent heat vaporisation (in the literature $L = 2.5 \cdot 10^6 - 2300\, T_{water}$ is commonly used); $C_e = 1.32 \cdot 10^{-3}$ is the moisture transfer coefficient (or Dalton number); W_{2m} is the wind speed 2 m above the sea surface; Q_{water} is the water vapour density close to the surface; Q_{air} is the water vapour density in the atmosphere; a_1 and b_1 are user specified constants. The default values are $a_1 = 0.5$ and $b_1 = 0.9$.

Measurements of Q_{water} and Q_{air} are not directly available but the vapour density can be related to the vapour pressure as

$$Q_i = \frac{0.2167}{T_i + T_k} e_i \tag{2.105}$$

in which subscript *i* refers to both water and air. The vapour pressure close to the sea, e_{water}, can be expressed in terms of the water temperature assuming that the air close to the surface is saturated and has the same temperature as the water

$$e_{water} = 6.11 e^{K\left(\frac{1}{T_k} - \frac{1}{T_{water} + T_k}\right)} \tag{2.106}$$

where $K = 5418\,°K$ and $T_K = 273.15\,°K$ is the temperature at 0 C. Similarly the vapour pressure of the air, e_{air}, can be expressed in terms of the air temperature and the relative humidity, R

$$e_{air} = R \cdot 6.11 e^{K\left(\frac{1}{T_k} - \frac{1}{T_{air} + T_k}\right)} \tag{2.107}$$

Replacing Q_{water} and Q_{air} with these expressions the latent heat can be written as

$$q_v = -P_v\left(a_1 + b_1 W_{2m}\right) \cdot \left(\frac{\exp\left(K\left(\frac{1}{T_k} - \frac{1}{T_{water} + T_k}\right)\right)}{T_{water} + T_k} - \frac{R \cdot \exp\left(K\left(\frac{1}{T_k} - \frac{1}{T_{air} + T_k}\right)\right)}{T_{air} + T_k} \right) \tag{2.108}$$

where all constants have been included in a new latent constant $P_v = 4370$ J $\cdot °K / m^3$. During cooling of the surface the latent heat loss has a major effect with typical values up to 100 W/m^2.

The wind speed, W_2, 2 m above the sea surface is calculated from the from the wind speed, W_{10}, 10 m above the sea surface using the following formula:

Assuming a logarithmic profile the wind speed, *u(z),* at a distance *z* above the sea surface is given by

$$u(z) = \frac{u_*}{\kappa} \log\left(\frac{z}{z_o}\right) \tag{2.109}$$

where u_* is the wind friction velocity, z_0 is the sea roughness and κ =0.4 is von Karman's constant. u_* and z_0 are given by

$$z_0 = z_{Charnock} u_*^2 / g \tag{2.110}$$

$$u_* = \frac{\kappa u(z)}{\log\left(\frac{z}{z_0}\right)} \tag{2.111}$$

where $z_{Charnock}$ is the Charnock parameter. The default value is $z_{Charnock} = 0.014$. The wind speed, W_2, 2 m above the sea surface is then calculated from the from the wind speed, W_{10}, 10m above the sea surface by first solving Eq. (2.114) and Eq. (2.115) iteratively for z_0 with $z=10m$ and $u(z)=W_{10}$. Then W_2 is given by

$$W_2 = W_{10} \frac{\log\left(\frac{2}{z_o}\right)}{\log\left(\frac{10}{z_0}\right)} \qquad W_{10} > 0.5 m/s$$
$$W_2 = W_{10} \qquad W_{10} \le 0.5 m/s \tag{2.112}$$

The heat loss due to vaporization occurs both by wind driven forced convection by and free convection. The effect of free convection is taken into account by the parameter a_1 in Eq. (2.104). The free convection is also taken into account by introducing a critical wind speed $W_{critical}$ so that the wind speed used in Eq. (2.112) is obtained as $W_{10}=max(W_{10},W_{critical})$. The default value for the critical wind speed is 2 m/s.

2.10.2 Convection

The sensible heat flux, q_c (W/m^2), (or the heat flux due to convection) depends on the type of boundary layer between the sea surface and the atmosphere. Generally this boundary layer is turbulent implying the following relationship

$$q_c = \begin{cases} \rho_{air} c_{air} c_{heating} W_{10} (T_{air} - T_{water}) & T_{air} \ge T \\ \rho_{air} c_{air} c_{cooling} W_{10} (T_{air} - T_{water}) & T_{air} < T \end{cases} \tag{2.113}$$

where ρ_{air} is the air density 1.225 kg/m^3; $c_{air} = 1007\ J/(kg \cdot °K)$ is the specific heat of air; $c_{heating} = 0.0011$ and $c_{cooling} = 0.0011$, respectively, is the sensible transfer coefficient (or Stanton number) for heating and cooling (see Kantha and Clayson, 2000); W_{10} is the wind speed 10 m above the sea surface; T_{water} is the temperature at the sea surface; T_{air} is the temperature of the air.

The convective heat flux typically varies between 0 and 100 W/m^2.

The heat loss due to convection occurs both by wind driven forced convection by and free convection. The free convection is taken into account by introducing a critical wind speed $W_{critical}$ so that the wind speed used in Eq. (2.113) is obtained as $W_{10}=max(W_{10},W_{critical})$. The default value for the critical wind speed is 2 m/s.

2.10.3 Short wave radiation

Radiation from the sun consists of electromagnetic waves with wave lengths varying from 1,000 to 30,000 Å. Most of this is absorbed in the ozone layer, leaving only a fraction of the energy to reach the surface of the Earth. Furthermore, the spectrum changes when sunrays pass through the atmosphere. Most of the infrared and ultraviolet compound is absorbed such that the solar radiation on the Earth mainly consists of light with wave lengths between 4,000 and 9,000 Å. This radiation is normally termed short wave radiation. The intensity depends on the distance to the sun, declination angle and latitude, extraterrestrial radiation and the cloudiness and amount of water vapour in the atmosphere (see Iqbal, 1983)

The eccentricity in the solar orbit, E_0, is given by

$$E_0 = \left(\frac{r_0}{r}\right)^2 = 1.000110 + 0.034221\cos(\Gamma) + 0.001280\sin(\Gamma) + 0.000719\cos(2\Gamma) + 0.000077\sin(2\Gamma) \quad (2.114)$$

where r_0 is the mean distance to the sun, r is the actual distance and the day angle $\Gamma\ (rad)$ is defined by

$$\Gamma = \frac{2\pi(d_n - 1)}{365} \quad (2.115)$$

and d_n is the Julian day of the year.

The daily rotation of the Earth around the polar axes contributes to changes in the solar radiation. The seasonal radiation is governed by the declination angle, $\delta\ (rad)$, which can be expressed by

$$\delta = 0.006918 - 0.399912\cos(\Gamma) + 0.07257\sin(\Gamma) - 0.006758\cos(2\Gamma) + 0.000907\sin(2\Gamma) - 0.002697\cos(3\Gamma) + 0.00148\sin(3\Gamma) \quad (2.116)$$

The day length, n_d, varies with δ. For a given latitude, ϕ, (positive on the northern hemisphere) the day length is given by

$$n_d = \frac{24}{\pi}\arccos\left(-\tan(\phi)\tan(\delta)\right) \tag{2.117}$$

and the sunrise angle, $\omega_{sr}\ (rad)$, and the sunset angle $\omega_{ss}\ (rad)$ are

$$\omega_{sr} = \arccos\left(-\tan(\phi)\tan(\delta)\right) \quad \text{and} \quad \omega_{ss} = -\omega_{sr} \tag{2.118}$$

The intensity of short wave radiation on the surface parallel to the surface of the Earth changes with the angle of incidence. The highest intensity is in zenith and the lowest during sunrise and sunset. Integrated over one day the extraterrestrial intensity, $H_0\ (MJ/m^2/day)$, in short wave radiation on the surface can be derived as

$$H_0 = \frac{24}{\pi} q_{sc} E_0 \cos(\phi)\cos(\delta)\left(\sin(\omega_{sr}) - \omega_{sr}\cos(\omega_{sr})\right) \tag{2.119}$$

where $q_{sc} = 4.9212\ (MJ/m^2/h)$ is the solar constant.

For determination of daily radiation under cloudy skies, $H\ (MJ/m^2/day)$, the following relation is used

$$\frac{H}{H_0} = a_2 + b_2\frac{n}{n_d} \tag{2.120}$$

in which n is the number of sunshine hours and n_d is the maximum number of sunshine hours. a_2 and b_2 are user specified constants. The default values are $a_2 = 0.295$ and $b_2 = 0.371$. The user-specified clearness coefficient corresponds to n/n_d. Thus the solar radiation, $q_s\ (W/m^2)$, can be expressed as

$$q_s = \left(\frac{H}{H_0}\right) q_0\left(a_3 + b_3\cos(\omega_i)\right)\frac{10^6}{3600} \tag{2.121}$$

where

$$a_3 = 0.4090 + 0.5016\sin\left(\omega_{sr} - \frac{\pi}{3}\right) \tag{2.122}$$

$$b_3 = 0.6609 + 0.4767\sin\left(\omega_{sr} - \frac{\pi}{3}\right) \tag{2.123}$$

The extraterrestrial intensity, $q_0\ (MJ/m^2/h)$ and the hour angle ω_i is given by

$$q_0 = q_{sc} E_0 \left(\sin(\phi)\sin(\delta) + \frac{24}{\pi}\cos(\phi)\cos(\delta)\cos(\omega_i) \right) \quad (2.124)$$

$$\omega_i = \frac{\pi}{12}\left(12 + \Delta t_{displacement} + \frac{4}{60}(L_S - L_E) - \frac{E_t}{60} - t_{local} \right) \quad (2.125)$$

$\Delta t_{displacement}$ is the displacement hours due to summer time and the time meridian L_S is the standard longitude for the time zone. $\Delta t_{displacement}$ and L_S are user specified constants. The default values are $\Delta t_{displacement} = 0\ (h)$ and $L_S = 0\ (deg)$. L_E is the local longitude in degrees. $E_t\ (s)$ is the discrepancy in time due to solar orbit and is varying during the year. It is given by

$$E_t = \begin{pmatrix} 0.000075 + 0.001868\cos(\Gamma) - 0.032077\sin(\Gamma) \\ -0.014615\cos(2\Gamma) - 0.04089\sin(2\Gamma) \end{pmatrix} \cdot 229.18 \quad (2.126)$$

Finally, t_{local} is the local time in hours.

Solar radiation that impinges on the sea surface does not all penetrate the water surface. Parts are reflected back and are lost unless they are backscattered from the surrounding atmosphere. This reflection of solar energy is termed the albedo. The amount of energy, which is lost due to albedo, depends on the angle of incidence and angle of refraction. For a smooth sea the reflection can be expressed as

$$\alpha = \frac{1}{2}\left(\frac{\sin^2(i-r)}{\sin^2(i+r)} + \frac{\tan^2(i-r)}{\tan^2(i+r)} \right) \quad (2.127)$$

where *i* is the angle of incidence, *r* the refraction angle and α the reflection coefficient, which typically varies from 5 to 40 %. α can be approximated using

$$\alpha = \begin{cases} \frac{altitude}{5}\,0.48 & altitude < 5 \\ \frac{30 - altitude}{25}(0.48 - 0.05) & 5 \le altitude \le 30 \\ 0.05 & altitude > 30 \end{cases} \quad (2.128)$$

where the altitude in degrees is given by

$$altitude = 90 - \left(\frac{180}{\pi}\arccos(\sin(\delta)\sin(\phi) + \cos(\delta)\cos(\phi)\cos(\omega_i)) \right) \quad (2.129)$$

Thus the net short wave radiation, $q_{s,net}\ (W/m^2)$, can possibly be expressed as

$$q_{sr,net} = (1-\alpha)q_s \quad (2.130)$$

The net short wave radiation, $q_{sr,net}$, can be calculated using empirical formulae as described above. Alternatively, the net short wave radiation can be calculated using Eq. (2.130) where the solar radiation, q_s, is specified by the user or the net short wave radiation, $q_{sr,net}$, can be given by the user.

2.10.4 Long wave radiation

A body or a surface emits electromagnetic energy at all wavelengths of the spectrum. The long wave radiation consists of waves with wavelengths between 9,000 and 25,000 Å. The radiation in this interval is termed infrared radiation and is emitted from the atmosphere and the sea surface. The long wave emittance from the surface to the atmosphere minus the long wave radiation from the atmosphere to the sea surface is called the net long wave radiation and is dependent on the cloudiness, the air temperature, the vapour pressure in the air and the relative humidity. The net outgoing long wave radiation, $q_{lr,net}\ (W/m^2)$, is given by Brunt's equation (See Lind and Falkenmark, 1972)

$$q_{lr,net} = -\sigma_{sb}\left(T_{air} + T_K\right)^4\left(a - b\sqrt{e_d}\right)\left(c + d\frac{n}{n_d}\right) \tag{2.131}$$

where e_d is the vapour pressure at dew point temperature measured in *mb*; n is the number of sunshine hours, n_d is the maximum number of sunshine hours; $\sigma_{sb} = 5.6697 \cdot 10^{-8}\ W/(m^2 \cdot {}^\circ K^4)$ is Stefan Boltzman's constant; $T_{air}\ (°C)$ is the air temperature. The coefficients *a*, *b*, *c* and *d* are given as

$$a = 0.56; b = 0.077 mb^{-1/2}; c = 0.10; d = .90 \tag{2.132}$$

The vapour pressure is determined as

$$e_d = 10 \cdot R\, e_{saturated} \tag{2.133}$$

where *R* is the relative humidity and the saturated vapour pressure, $e_{saturated}\ (kPa)$, with 100 % relative humidity in the interval from –51 to 52 °C can be estimated by

$$e_{saturated} = 3.38639 \cdot \left(\left(7.38 \cdot 10^{-3} \cdot T_{air} + 0.8072\right)^8 - 1.9 \cdot 10^{-5}\left|1.8 \cdot T_{air} + 48\right| + 1.316 \cdot 10^{-3}\right) \tag{2.134}$$

The net long wave radiation, $q_{lr,net}$, can be calculated using empirical formulae as described above. Alternatively, the net long wave radiation can be calculated as

$$q_{lr,net} = q_{ar,net} - q_{br} \tag{2.135}$$

where the net incident atmospheric radiation, $q_{ar,net}$, is specified by the user and the back radiation, q_{br}, is given by

$$q_{br} = (1 - r)\varepsilon\sigma_{sb}T_K^4 \tag{2.136}$$

where r=0.03 is the reflection coefficient and ε=0.985 is the emissivity factor of the atmosphere. The net long wave radiation can also be specified by the user.

3 Numerical Solution

3.1 Spatial Discretization

The discretization in solution domain is performed using a finite volume method. The spatial domain is discretized by subdivision of the continuum into non-overlapping cells/elements.

In the two-dimensional case the elements can be arbitrarily shaped polygons, however, here only triangles and quadrilateral elements are considered.

In the three-dimensional case a layered mesh is used: in the horizontal domain an unstructured mesh is used while in the vertical domain a structured mesh is used (see Figure 3.1). The vertical mesh is based on either sigma coordinates or combined sigma/z-level coordinates. For the hybrid sigma/z-level mesh sigma coordinates are used from the free surface to a specified depth and z-level coordinates are used below. The different types of vertical mesh are illustrated in Figure 3.2. The elements in the sigma domain and the z-level domain can be prisms with either a 3-sided or 4-sided polygonal base. Hence, the horizontal faces are either triangles or quadrilateral element. The elements are perfectly vertical and all layers have identical topology.

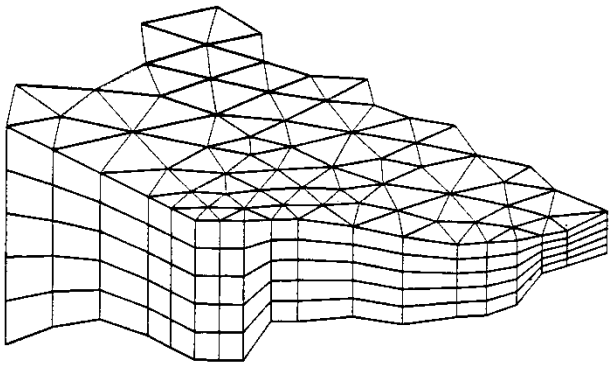

Figure 3.1 Principle of meshing for the three-dimensional case

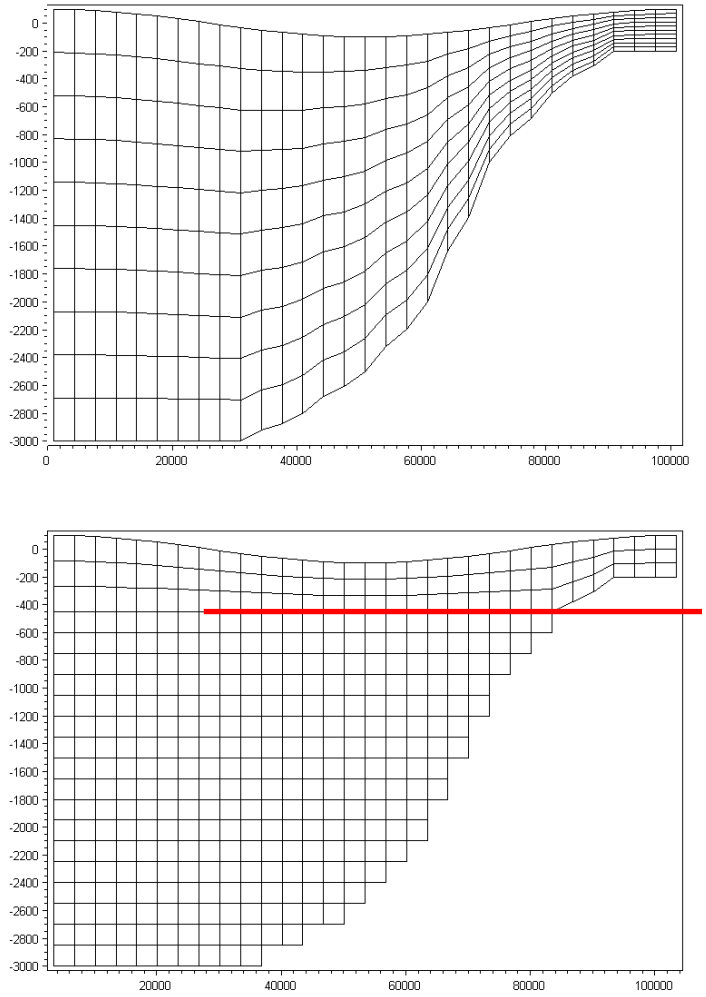

Figure 3.2 Illustrations of the different vertical grids. Upper: sigma mesh, Lower: combined sigma/z-level mesh with simple bathymetry adjustment. The red line shows the interface between the z-level domain and the sigma-level domain

The most important advantage using sigma coordinates is their ability to accurately represent the bathymetry and provide consistent resolution near the bed. However, sigma coordinates can suffer from significant errors in the horizontal pressure gradients, advection and mixing terms in areas with sharp topographic changes (steep slopes). These errors can give rise to unrealistic flows.

The use of z-level coordinates allows a simple calculation of the horizontal pressure gradients, advection and mixing terms, but the disadvantages are their inaccuracy in representing the bathymetry and that the stair-step representation of the bathymetry can result in unrealistic flow velocities near the bottom.

3.1.1 Vertical Mesh

For the vertical discretization both a standard sigma mesh and a combined sigma/z-level mesh can be used. For the hybrid sigma/z-level mesh sigma coordinates are used from the free surface to a specified depth, z_σ, and z-level coordinates are used below. At least one sigma layer is needed to allow changes in the surface elevation.

Sigma

In the sigma domain a constant number of layers, N_σ, are used and each sigma layer is a fixed fraction of the total depth of the sigma layer, h_σ, where $h_\sigma = \eta - \max(z_b, z_\sigma)$. The discretization in the sigma domain is given by a number of discrete σ-levels $\{\sigma_i,\ \ i = 1, (N_\sigma + 1)\}$. Here σ varies from $\sigma_1 = 0$ at the bottom interface of the lowest sigma layer to $\sigma_{N_\sigma+1} = 1$ at the free surface.

Variable sigma coordinates can be obtained using a discrete formulation of the general vertical coordinate (s-coordinate) system proposed by Song and Haidvogel (1994). First an equidistant discretization in a s-coordinate system *(-1≤ s ≤0)* is defined

$$s_i = -\frac{N_\sigma + 1 - i}{N_\sigma} \qquad i = 1, (N_\sigma + 1) \tag{3.1}$$

The discrete sigma coordinates can then be determined by

$$\sigma_i = 1 + \sigma_c s_i + (1 - \sigma_c) c(s_i) \quad i = 1, (N_\sigma + 1) \tag{3.2}$$

where

$$c(s) = (1 - b)\frac{\sinh(\theta s)}{\sinh(\theta)} + b\frac{\tanh\left(\theta\left(s + \frac{1}{2}\right)\right) - \tanh(\frac{\theta}{2})}{2\tanh(\frac{\theta}{2})} \tag{3.3}$$

Here σ_c is a weighting factor between the equidistant distribution and the stretch distribution, θ is the surface control parameter and b is the bottom control parameter. The range for the weighting factor is $0<\sigma_c\leq 1$ where the value 1 corresponds to equidistant distribution and 0 corresponds to stretched distribution. A small value of σ_c can result in linear instability. The range of the surface control parameter is $0<\theta\leq 20$ and the range of the bottom control parameter is $0\leq b\leq 1$. If $\theta<<1$ and $b=0$ an equidistant vertical resolution is obtained. By increasing the value of the θ, the highest resolution is achieved near the surface. If $\theta>0$ and $b=1$ a high resolution is obtained both near the surface and near the bottom.

Examples of a mesh using variable vertical discretization are shown in Figure 3.3 and Figure 3.4.

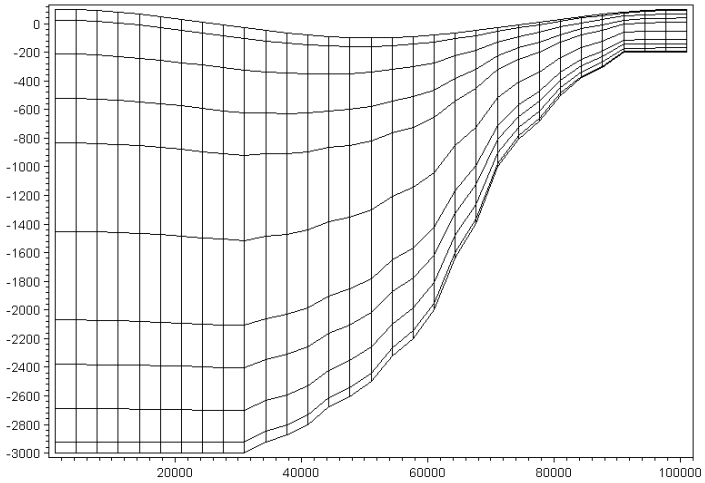

Figure 3.3 Example of vertical distribution using layer thickness distribution. Number of layers: 10, thickness of layers 1 to 10: .025, 0.075, 0.1, 0.01, 0.02, 0.02, 0.1, 0.1, 0.075, 0.025

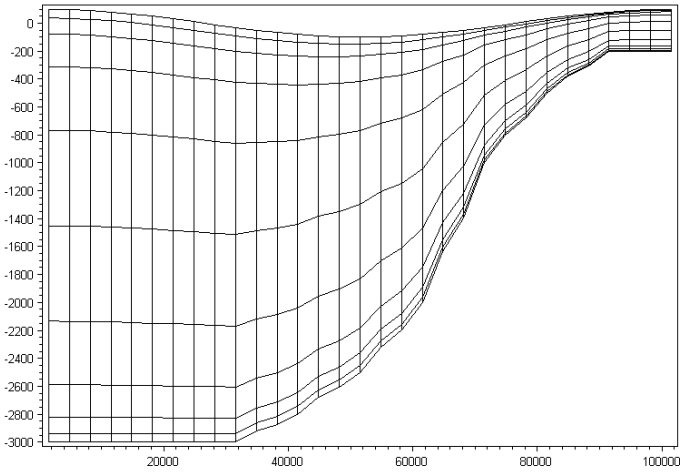

Figure 3.4 Example of vertical distribution using variable distribution. Number of layers: 10, σ_c = 0.1, θ = 5, b = 1

Combined sigma/z-level

In the z-level domain the discretization is given by a number of discrete z-levels $\{z_i,\ i = 1, (N_z + 1)\}$, where N_z is the number of layers in the z-level domain. z_1 is the minimum z-level and z_{N_z+1} is the maximum z-level, which is equal to the sigma depth, z_σ. The corresponding layer thickness is given by

$$\Delta z_i = z_{i+1} - z_i \qquad i = 1, N_z \tag{3.4}$$

The discretization is illustrated in Figure 3.5 and Figure 3.6.

Using standard z-level discretization the bottom depth is rounded to the nearest z-level. Hence, for a cell in the horizontal mesh with the cell-averaged depth, z_b, the cells in the corresponding column in the z-domain are included if the following criteria is satisfied

$$(z_{i+1} - z_i)/2 \geq z_b \quad i = 1, N_z \tag{3.5}$$

The cell-averaged depth, z_b, is calculated as the mean value of the depth at the vortices of each cell. For the standard z-level discretization the minimum depth is given by z_1. Too take into account the correct depth for the case where the bottom depth is below the minimum z-level ($z_1 > z_b$) a bottom fitted approach is used. Here, a correction factor, f_1, for the layer thickness in the bottom cell is introduced. The correction factor is used in the calculation of the volume and face integrals. The correction factor for the bottom cell is calculated by

$$f_1 = \frac{(z_2 - z_b)}{\Delta z_1} \tag{3.6}$$

The corrected layer thickness is given by $\Delta z_1^* = f_1 \Delta z_1$. The simple bathymetry adjustment approach is illustrated in Figure 3.5.

For a more accurate representation of the bottom depth an advanced bathymetry adjustment approach can be used. For a cell in the horizontal mesh with the cell-averaged depth, z_b, the cells in the corresponding column in the z-domain are included if the following criteria is satisfied

$$z_{i+1} > z_b \qquad i = 1, N_z \tag{3.7}$$

A correction factor, f_i, is introduced for the layer thickness

$$\begin{aligned} f_i &= max\left(\frac{(z_{i+1} - z_b)}{\Delta z_i}, \frac{z_{min}}{\Delta z_i}\right) && z_i < z_b < z_{i+1} \;\; or \;\; z_1 > z_b \\ f_i &= 1 && z_1 \geq z_b \end{aligned} \tag{3.8}$$

A minimum layer thickness, Δz_{min}, is introduced to avoid very small values of the correction factor. The correction factor is used in the calculation of the volume and face integrals. The corrected layer thicknesses are given by $\{\Delta z_i^* = f_i \Delta z_i, \; i = 1, N_z\}$. The advanced bathymetry adjustment approach is illustrated in Figure 3.6.

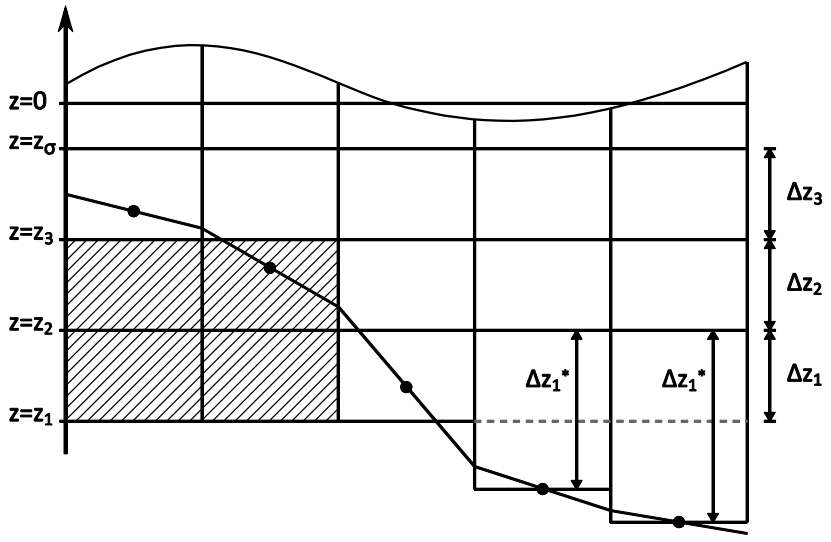

Figure 3.5 Simple bathymetry adjustment approach

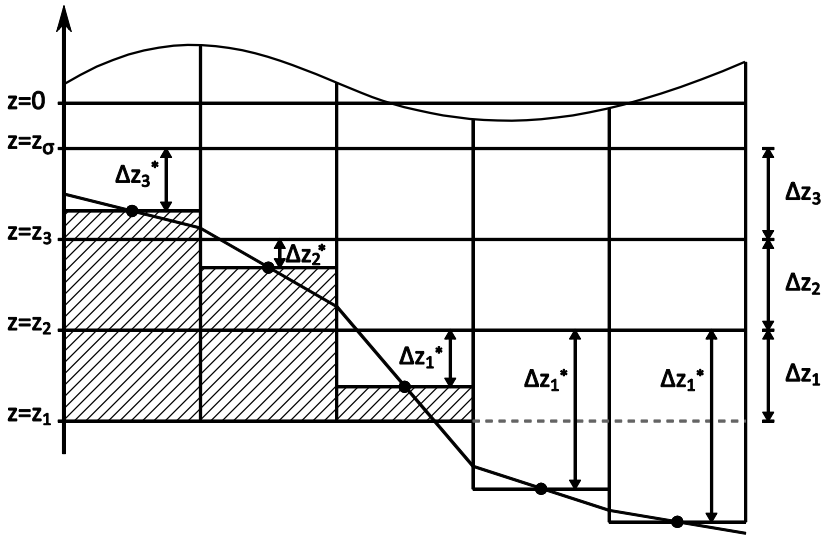

Figure 3.6 Advanced bathymetry adjustment approach

3.1.2 Shallow water equations

The integral form of the system of shallow water equations can in general form be written

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U}) \tag{3.9}$$

where ***U*** is the vector of conserved variables, ***F*** is the flux vector function and ***S*** is the vector of source terms.

In Cartesian coordinates the system of 2D shallow water equations can be written

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \left(\mathbf{F}_x^I - \mathbf{F}_x^V\right)}{\partial x} + \frac{\partial \left(\mathbf{F}_y^I - \mathbf{F}_y^V\right)}{\partial y} = \mathbf{S} \tag{3.10}$$

where the superscripts *I* and *V* denote the inviscid (convective) and viscous fluxes, respectively and where

$$\mathbf{U} = \begin{bmatrix} h \\ h\bar{u} \\ h\bar{v} \end{bmatrix},$$

$$\mathbf{F}_x^{\,I} = \begin{bmatrix} h\bar{u} \\ h\bar{u}^2 + \frac{1}{2}g(h^2 - d^2) \\ h\bar{u}\bar{v} \end{bmatrix}, \quad F_x^{\,V} = \begin{bmatrix} 0 \\ hA\left(2\frac{\partial \bar{u}}{\partial x}\right) \\ hA\left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x}\right) \end{bmatrix}$$

$$\mathbf{F}_y^{\,I} = \begin{bmatrix} h\bar{v} \\ h\bar{v}\bar{u} \\ h\bar{v}^2 + \frac{1}{2}g(h^2 - d^2) \end{bmatrix}_a, \quad F_y^{\,V} = \begin{bmatrix} 0 \\ hA\left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x}\right) \\ hA\left(2\frac{\partial \bar{v}}{\partial x}\right) \end{bmatrix} \tag{3.11}$$

$$\mathbf{S} = \begin{bmatrix} 0 \\ g\eta\frac{\partial d}{\partial x} + f\bar{v}h - \frac{h}{\rho_0}\frac{\partial p_a}{\partial x} - \frac{gh^2}{2\rho_0}\frac{\partial \rho}{\partial x} - \frac{1}{\rho_0}\left(\frac{\partial s_{xx}}{\partial x} + \frac{\partial s_{xy}}{\partial y}\right) \\ \qquad + \frac{\tau_{sx}}{\rho_0} - \frac{\tau_{bx}}{\rho_0} + hu_s \\ g\eta\frac{\partial d}{\partial y} - f\bar{u}h - \frac{h}{\rho_0}\frac{\partial p_a}{\partial y} - \frac{gh^2}{2\rho_0}\frac{\partial \rho}{\partial y} - \frac{1}{\rho_0}\left(\frac{\partial s_{yx}}{\partial x} + \frac{\partial s_{yy}}{\partial y}\right) \\ \qquad + \frac{\tau_{sy}}{\rho_0} - \frac{\tau_{by}}{\rho_0} + hv_s \end{bmatrix}$$

In Cartesian coordinates the system of 3D shallow water equations can be written

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_x^{\,I}}{\partial x'} + \frac{\partial \mathbf{F}_y^{\,I}}{\partial y'} + \frac{\partial \mathbf{F}_\sigma^{\,I}}{\partial \sigma} + \frac{\partial \mathbf{F}_x^{\,V}}{\partial x} + \frac{\partial \mathbf{F}_y^{\,V}}{\partial y} + \frac{\partial \mathbf{F}_\sigma^{\,V}}{\partial \sigma} = \mathbf{S} \tag{3.12}$$

where the superscripts *I* and *V* denote the inviscid (convective) and viscous fluxes, respectively and where

$$\mathbf{U} = \begin{bmatrix} h \\ hu \\ hv \end{bmatrix},$$

$$\mathbf{F}_x^{\,I} = \begin{bmatrix} h\bar{u} \\ hu^2 + \frac{1}{2}g(h^2 - d^2) \\ huv \end{bmatrix}, \quad \mathbf{F}_x^{\,V} = \begin{bmatrix} 0 \\ hA\left(2\frac{\partial u}{\partial x}\right) \\ hA\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \end{bmatrix}$$

$$\mathbf{F}_y^{\,I} = \begin{bmatrix} h\bar{v} \\ hvu \\ hv^2 + \frac{1}{2}g(h^2 - d^2) \end{bmatrix}, \quad \mathbf{F}_y^{\,V} = \begin{bmatrix} 0 \\ hA\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \\ hA\left(2\frac{\partial v}{\partial x}\right) \end{bmatrix} \tag{3.13}$$

$$\mathbf{F}_\sigma^{\,I} = \begin{bmatrix} h\omega \\ h\omega u \\ h\omega v \end{bmatrix}, \quad \mathbf{F}_\sigma^{\,V} = \begin{bmatrix} 0 \\ \frac{\upsilon_t}{h}\frac{\partial u}{\partial \sigma} \\ \frac{\upsilon_t}{h}\frac{\partial v}{\partial \sigma} \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} 0 \\ g\eta\frac{\partial d}{\partial x} + fvh - \frac{h}{\rho_0}\frac{\partial p_a}{\partial x'} - \frac{hg}{\rho_0}\int_z^\eta \frac{\partial \rho}{\partial x}dz - \frac{1}{\rho_0}\left(\frac{\partial s_{xx}}{\partial x} + \frac{\partial s_{xy}}{\partial y}\right) + hu_s \\ g\eta\frac{\partial d}{\partial y} - fuh - \frac{h}{\rho_0}\frac{\partial p_a}{\partial y'} - \frac{hg}{\rho_0}\int_z^\eta \frac{\partial \rho}{\partial y}dz - \frac{1}{\rho_0}\left(\frac{\partial s_{yx}}{\partial x} + \frac{\partial s_{yy}}{\partial y}\right) + hv_s \end{bmatrix}$$

Integrating Eq. (3.9) over the *i*th cell and using Gauss's theorem to rewrite the flux integral gives

$$\int_{A_i}\frac{\partial \mathbf{U}}{\partial t}d\Omega + \int_{\Gamma_i}(\mathbf{F}\cdot\mathbf{n})\,ds = \int_{A_i}\mathbf{S}(\mathbf{U})d\Omega \tag{3.14}$$

where A_i is the area/volume of the cell Ω is the integration variable defined on A_i, Γ_i is the boundary of the *i*th cell and *ds* is the integration variable along the boundary. ***n*** is the unit outward normal vector along the boundary. Evaluating the area/volume integrals by a one-point quadrature rule, the quadrature point being the centroid of the cell, and evaluating the boundary intergral using a mid-point quadrature rule, Eq. (3.14) can be written

$$\frac{\partial U_i}{\partial t} + \frac{1}{A_i}\sum_j^{NS} \mathbf{F}\cdot\mathbf{n}\,\Delta\Gamma_j = S_i \tag{3.15}$$

Here U_i and S_i, respectively, are average values of U and S over the *i*th cell and stored at the cell centre, NS is the number of sides of the cell, n_j is the unit outward normal vector at the *j*th side and $\Delta\Gamma_j$ the length/area of the *j*th interface.

Both a first order and a second order scheme can be applied for the spatial discretization.

For the 2D case an approximate Riemann solver (Roe's scheme, see Roe, 1981) is used to calculate the convective fluxes at the interface of the cells. Using the Roe's scheme the dependent variables to the left and to the right of an interface have to be estimated. Second-order spatial accuracy is achieved by employing a linear gradient-reconstruction technique. The average gradients are estimated using the approach by Jawahar and Kamath, 2000. To avoid numerical oscillations a second order TVD slope limiter (Van Leer limiter, see Hirch, 1990 and Darwish, 2003) is used.

For the 3D case an approximate Riemann solver (Roe's scheme, see Roe, 1981) is used to calculate the convective fluxes at the vertical interface of the cells (x'y'-plane). Using the Roe's scheme the dependent variables to the left and to the right of an interface have to be estimated. Second-order spatial accuracy is achieved by employing a linear gradient-reconstruction technique. The average gradients are estimated using the approach by Jawahar and Kamath, 2000. To avoid numerical oscillations a second order TVD slope limiter (Van Leer limiter, see Hirch, 1990 and Darwish, 2003) is used. The convective fluxes at the horizontal interfaces (vertical line) are derived using first order upwinding for the low order scheme. For the higher order scheme the fluxes are approximated by the mean value of the fluxes calculated based on the cell values above and below the interface for the higher order scheme.

3.1.3 Transport equations

The transport equations arise in the salt and temperature model, the turbulence model and the generic transport model. They all share the form of Equation Eq. (2.20) in Cartesian coordinates. For the 2D case the integral form of the transport equation can be given by Eq. (3.9) where

$$\mathbf{U} = h\bar{C}$$

$$\mathbf{F}^I = \left[h\bar{u}\bar{C},\quad h\bar{v}\bar{C}\right]$$

$$\mathbf{F}^V = \left[hD_h\frac{\partial\bar{C}}{\partial x},\quad hD_h\frac{\partial\bar{C}}{\partial y}\right] \tag{3.16}$$

$$\mathbf{S} = -hk_p\bar{C} + hC_sS.$$

For the 3D case the integral form of the transport equation can be given by Eq. (3.9) where

$$\mathbf{U} = \mathrm{hC}$$

$$\mathbf{F}^{\mathrm{I}} = \left[\mathrm{huC},\quad \mathrm{hvC},\quad \mathrm{h}\omega\mathrm{C}\right]$$
$$\mathbf{F}^{\mathrm{V}} = \left[\mathrm{hD_h}\partial\frac{\partial \mathrm{C}}{\partial \mathrm{x}},\quad \mathrm{hD_h}\partial\frac{\partial \mathrm{C}}{\partial \mathrm{y}},\quad \mathrm{h}\frac{\mathrm{D_h}}{\mathrm{h}}\partial\frac{\partial \mathrm{C}}{\partial \sigma}\right] \tag{3.17}$$

$$\mathbf{S} = -\mathrm{hk_p C} + \mathrm{hC_s S}.$$

The discrete finite volume form of the transport equation is given by Eq. (3.15). As for the shallow water equations both a first order and a second order scheme can be applied for the spatial discretization.

In 2D the low order approximation uses simple first order upwinding, i.e., element average values in the upwinding direction are used as values at the boundaries. The higher order version approximates gradients to obtain second order accurate values at the boundaries. Values in the upwinding direction are used. To provide stability and minimize oscillatory effects, a TVD-MUSCL limiter is applied (see Hirch, 1990, and Darwish, 2003).

In 3D the low order version uses simple first order upwinding. The higher order version approximates horizontal gradients to obtain second order accurate values at the horizontal boundaries. Values in the upwinding direction are used. To provide stability and minimize oscillatory effects, an ENO (Essentially Non-Oscillatory) type procedure is applied to limit the horizontal gradients. In the vertical direction a 3rd order ENO procedure is used to obtain the vertical face values (Shu, 1997).

3.2 Time Integration

Consider the general form of the equations

$$\frac{\partial \mathbf{U}}{\partial \mathrm{t}} = \mathbf{G}\left(\mathbf{U}\right) \tag{3.18}$$

For 2D simulations, there are two methods of time integration for both the shallow water equations and the transport equations: A low order method and a higher order method. The low order method is a first order explicit Euler method

$$\mathbf{U}_{\mathrm{n+1}} = \mathbf{U}_{\mathrm{n}} + \Delta\mathrm{t}\ \mathbf{G}(\mathbf{U}_{\mathrm{n}}) \tag{3.19}$$

where Δt is the time step interval. The higher order method uses a second order Runge Kutta method on the form:

$$\mathbf{U}_{\mathrm{n+\frac{1}{2}}} = \mathbf{U}_{\mathrm{n}} + \tfrac{1}{2}\Delta\mathrm{t}\ \mathbf{G}(\mathbf{U}_{\mathrm{n}})$$
$$\mathbf{U}_{\mathrm{n+1}} = \mathbf{U}_{\mathrm{n}} + \Delta\mathrm{t}\ \mathbf{G}(\mathbf{U}_{\mathrm{n+\frac{1}{2}}}) \tag{3.20}$$

For 3D simulations the time integration is semi-implicit. The horizontal terms are treated implicitly and the vertical terms are treated implicitly or partly explicitly and partly implicitly. Consider the equations in the general semi-implicit form.

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{G}_h(\mathbf{U}) + \mathbf{G}_v(\mathbf{BU}) = \mathbf{G}_h(\mathbf{U}) + \mathbf{G}_v^I(\mathbf{U}) + \mathbf{G}_v^V(\mathbf{U}) \tag{3.21}$$

where the h and v subscripts refer to horizontal and vertical terms, respectively, and the superscripts refer to invicid and viscous terms, respectively. As for 2D simulations, there is a lower order and a higher order time integration method.

The low order method used for the 3D shallow water equations can written as

$$\mathbf{U}_{n+1} - \tfrac{1}{2}\Delta t\left(\mathbf{G}_v(\mathbf{U}_{n+1}) + \mathbf{G}_v(\mathbf{U}_n)\right) = \mathbf{U}_n + \Delta t\ \mathbf{G}_h(\mathbf{U}_n) \tag{3.22}$$

The horizontal terms are integrated using a first order explicit Euler method and the vertical terms using a second order implicit trapezoidal rule. The higher order method can be written

$$\begin{aligned} \mathbf{U}_{n+1/2} - \tfrac{1}{4}\Delta t\ \left(\mathbf{G}_v(\mathbf{U}_{n+1/2}) + \mathbf{G}_v(\mathbf{U}_n)\right) &= \mathbf{U}_n + \tfrac{1}{2}\Delta t\ \mathbf{G}_h(\mathbf{U}_n) \\ \mathbf{U}_{n+1} - \tfrac{1}{2}\Delta t\ \left(\mathbf{G}_v(\mathbf{U}_{n+1}) + \mathbf{G}_v(\mathbf{U}_n)\right) &= \mathbf{U}_n + \Delta t\ \mathbf{G}_h(\mathbf{U}_{n+1/2}) \end{aligned} \tag{3.23}$$

The horizontal terms are integrated using a second order Runge Kutta method and the vertical terms using a second order implicit trapezoidal rule.

The low order method used for the 3D transport equation can written as

$$\mathbf{U}_{n+1} - \tfrac{1}{2}\Delta t\left(\ \mathbf{G}_v^V(\mathbf{U}_{n+1}) + \mathbf{G}_v^V(\mathbf{U}_n)\right) = \mathbf{U}_n + \Delta t\ \mathbf{G}_h(\mathbf{U}_n) + \Delta t\ \mathbf{G}_v^I(\mathbf{U}_n) \tag{3.24}$$

The horizontal terms and the vertical convective terms are integrated using a first order explicit Euler method and the vertical viscous terms are integrated using a second order implicit trapezoidal rule. The higher order method can be written

$$\begin{aligned} \mathbf{U}_{n+1/2} - \tfrac{1}{4}\Delta t\ \left(\mathbf{G}_v^V(\mathbf{U}_{n+1/2}) + \mathbf{G}_v^V(\mathbf{U}_n)\right) = \\ \mathbf{U}_n + \tfrac{1}{2}\Delta t\ \mathbf{G}_h(\mathbf{U}_n) + \tfrac{1}{2}\Delta t\ \mathbf{G}_v^I(\mathbf{U}_n) \\ \mathbf{U}_{n+1} - \tfrac{1}{2}\Delta t\ \left(\mathbf{G}_v^V(\mathbf{U}_{n+1}) + \mathbf{G}_v^V(\mathbf{U}_n)\right) = \\ \mathbf{U}_n + \Delta t\ \mathbf{G}_h(\mathbf{U}_{n+1/2}) + \Delta t\ \mathbf{G}_v^I(\mathbf{U}_{n+1/2}) \end{aligned} \tag{3.25}$$

The horizontal terms and the vertical convective terms are integrated using a second order Runge Kutta method and the vertical terms are integrated using a second order implicit trapezoidal rule for the vertical terms.

3.3 Boundary Conditions

3.3.1 Closed boundaries

Along closed boundaries (land boundaries), normal fluxes are forced to zero for all variables. For the momentum equations, this leads to full-slip along land boundaries. For the shallow water equations, the no slip condition can also be applied where both the normal and tangential velocity components are zero.

3.3.2 Open boundaries

For the shallow water equations a number of different boundary conditions can be applied

The flux, velocity and Flather boundary conditions are all imposed using a weak approach. A ghost cell technique is applied where the primitive variables in the ghost cell are specified. The water level is evaluated based on the value of the adjacent interior cell, and the velocities are evaluated based on the boundary information. For a discharge boundary, the transverse velocity is set to zero for inflow and passively advected for outflow. The boundary flux is then calculated using an approximate Riemann solver.

The Flather (1976) condition is one of the most efficient open boundary conditions. It is very efficient in connection with downscaling coarse model simulations to local areas (see Oddo and Pinardi (2007)). The instabilities, which are often observed when imposing stratified density at a water level boundary, can be avoided using Flather conditions

The level boundary is imposed using a strong approach based on the characteristic theory (see e.g. Sleigh et al., 1998).

The discharge boundary condition is imposed using both a weak formulation using ghost cell technique described above and a strong approach based on the characteristic theory (see e.g. Sleigh et al., 1998).

Note that using the weak formulation for a discharge boundary the effective discharge over the boundary may deviate from the specified discharge.

For transport equations, either a specified value or a zero gradient can be given. For specified values, the boundary conditions are imposed by applying the specified concentrations for calculation of the boundary flux. For a zero gradient condition, the concentration at the boundary is assumed to be identical to the concentration at the adjacent interior cell.

3.3.3 Flooding and drying

The approach for treatment of the moving boundaries problem (flooding and drying fronts) is based on the work by Zhao et al. (1994) and Sleigh et al. (1998). When the depths are small the problem is reformulated and only when the depths are very small the elements/cells are removed from the calculation. The reformulation is made by setting the momentum fluxes to zero and only taking the mass fluxes into consideration.

The depth in each element/cell is monitored and the elements are classified as dry, partially dry or wet. Also the element faces are monitored to identify flooded boundaries.

- An element face is defined as flooded if the following two criteria are satisfied: Firstly, the water depth at one side of face must be less than a tolerance depth, h_{dry}, and the water depth at the other side of the face larger than a tolerance depth, h_{flood}. Secondly, the sum of the still water depth at the side for which the water depth is less than h_{dry} and the surface elevation at the other side must be larger than zero.
- An element is dry if the water depth is less than a tolerance depth, h_{dry}, and no of the element faces are flooded boundaries. The element is removed from the calculation.
- An element is partially dry if the water depth is larger than h_{dry} and less than a tolerance depth, h_{wet}, or when the depth is less than the h_{dry} and one of the element faces is a flooded boundary. The momentum fluxes are set to zero and only the mass fluxes are calculated.
- An element is wet if the water depth is greater than h_{wet}. Both the mass fluxes and the momentum fluxes are calculated.

The wetting depth, h_{wet}, must be larger than the drying depth, h_{dry}, and flooding depth, h_{flood}, must satisfy

$$h_{dry} < h_{flood} < h_{wet} \tag{3.26}$$

The default values are $h_{dry} = 0.005\,\mathrm{m}$, $h_{flood} = 0.05\,\mathrm{m}$ and $h_{wet} = 0.1\,\mathrm{m}$.

Note, that for very small values of the tolerance depth, h_{wet}, unrealistically high flow velocities can occur in the simulation and give cause to stability problems.

4 Infiltration and Leakage

The effect of infiltration and leakage at the surface zone may be important in cases of flooding scenarios on otherwise dry land. It is possible to account for this in one of two ways: by Net infiltration rates or by constant infiltration with capacity.

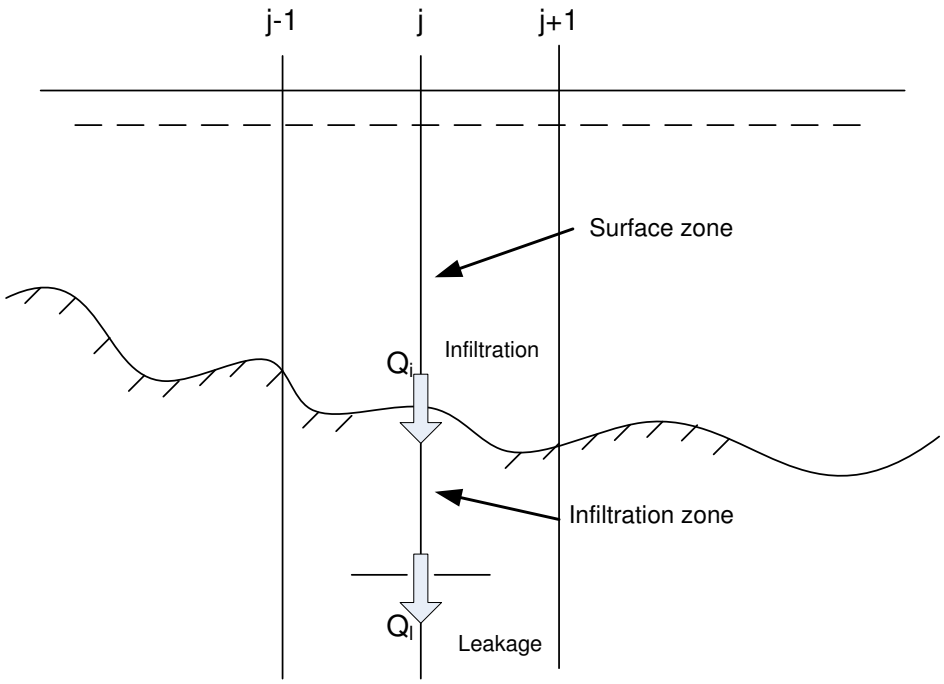

Figure 4.1 Illustration of infiltration process

4.1 Net Infiltration Rates

The net infiltration rate is defined directly. This will act as a simple sink in each element in the overall domain area.

The one-dimensional vertical continuity equation is solved at each hydrodynamic time step after the two-dimensional horizontal flow equations have been solved. The calculation of the new water depth in the free surface zone for each horizontal element is found by

$$H(j) = H(j) - V_{infiltration}(j) / A(j) \quad (4.1)$$

Where $V_{infiltration}(j)$ is the infiltrated volume in element (j) and A(j) the area of the element.

If $H(j)$ becomes marked as *dry* then element (j) will be taken out of the two-dimensional horizontal flow calculations and no infiltration can occur until the element is flooded again.

In summary: when using Net infiltration rate an unsaturated zone is never specified and thus has no capacity limits, so the specified infiltration rates will always be fully effectuated as long as there is enough water available in the element.

4.2 Constant Infiltration with Capacity

Constant infiltration with capacity describes the infiltration from the free surface zone to the unsaturated zone and from the unsaturated zone to the saturated zone by a simplified model. The model assumes the following:

- The unsaturated zone is modelled as an infiltration zone with constant porosity over the full depth of the zone.
- The flow between the free surface zone and the infiltration zone is based on a constant flow rate, i.e. $V_{infiltration} = Q_i \cdot \Delta t$ where Q_i is the prescribed flow rate.
- The flow between the saturated and unsaturated zone is modelled as a leakage Q_l having a constant flow rate, i.e. $V_{leakage} = Q_l \cdot \Delta t$.

The simplified model described above is solved through a one-dimensional continuity equation. Feedback from the infiltration and leakage to the two-dimensional horizontal hydrodynamic calculations is based solely on changes to the depth of the free surface zone – the water depth.

Note that the infiltration flow cannot exceed the amount of water available in the free surface water zone nor the difference between the water capacity of the infiltration zone and the actual amount of water stored there. It is possible that the infiltration flow completely drains the free surface zone from water and thus creates a dried-out point in the two-dimensional horizontal flow calculations.

The one-dimensional vertical continuity equation is solved at each hydrodynamic time step after the two-dimensional horizontal flow equations have been solved. The solution proceeds in the following way:

1. Calculation of the volume from leakage flow in each horizontal element – $V_{leakage}(j)$

$$V_{leakage}(j) = Q_l(j) \cdot \Delta t \cdot A(j) \tag{4.2}$$

$$V_{leakage}(j) = \min(V_{leakage}(j), V_i(j)) \tag{4.3}$$

$$V_i(j) := V_i(j) - V_{leakage}(j) \tag{4.4}$$

   Where $V_i(j)$ is the total amount of water in the infiltration zone and $Q_l(j)$ is the leakage flow rate.

2. Calculation of the volume from infiltration flow in each horizontal element – $V_{infiltration}(j)$

$$V_{infiltration}(j) = Q_i(j) \cdot \Delta t \cdot A(j) \tag{4.5}$$

$$V_{infiltration}(j) = \min\left(V_{infiltration}(j), SC_i(j) - V_i(j), H(j) \cdot A(j)\right) \tag{4.6}$$

$$V_i(j) := V_i(j) + V_{infiltration}(j) \tag{4.7}$$

Where $Q_i(j)$ is the infiltration rate, $SC_i(j)$ is the water storage capacity and $H(j)$ the depth of the free surface.

3. Calculation of the new water depth in the free surface zone for each horizontal element

$$H(j) = H(j) - V_{infiltration}(j)/A(j) \tag{4.8}$$

If $H(j)$ becomes marked as *dry* then element *(j)* will be taken out of the two-dimensional horizontal flow calculations. The element can still *leak* but no infiltration can occur until the element is flooded again.

The water storage capacity of the infiltration zone is calculated as

$$SC_i(j) = Z_i(j) \cdot A(j) \cdot \gamma(j) \tag{4.9}$$

Where $Z_i(j)$ is the depth of the infiltration zone and $\gamma(j)$ is the porosity of the same zone.

In summary, when using Constant infiltration with capacity there can be situations where the picture is altered and the rates are either only partially effectuated or not at all:

- If $= H(j) < H_{dry}$ on the surface (dry surface) => infiltration rate is not effectuated
- If: the water volume in the infiltration zone reaches the full capacity => infiltration rate is not effectuated
- If: the water volume is zero in the infiltration zone (the case in many initial conditions) => leakage rate is not effectuated
- Leakage volume must never eclipse the available water volume in the infiltration zone, if so we utilise the available water volume in infiltration zone as leakage volume
- Infiltration volume must never eclipse the available water volume on the surface, if so we utilise the available water on the surface as infiltration volume

5 Validation

The new finite-volume model has been successfully tested in a number of basic, idealised situations for which computed results can be compared with analytical solutions or information from the literature. The model has also been applied and tested in more natural geophysical conditions; ocean scale, inner shelves, estuaries, lakes and overland, which are more realistic and complicated than academic and laboratory tests. A detailed validation report is under preparation.

This chapter presents a comparison between numerical model results and laboratory measurements for a dam-break flow in an L-shaped channel.

Additional information on model validation and applications can be found here

http://www.mikepoweredbydhi.com/download/product-documentation

5.1 Dam-break Flow through Sharp Bend

The physical model to be studied combines a square-shaped upstream reservoir and an L-shaped channel. The flow will be essentially two-dimensional in the reservoir and at the angle between the two reaches of the L-shaped channel. However, there are numerical and experimental evidences that the flow will be mostly unidimensional in both rectilinear reaches. Two characteristics or the dam-break flow are of special interest, namely

- The "damping effect" of the corner
- The upstream-moving hydraulic jump which forms at the corner

The multiple reflections of the expansion wave in the reservoir will also offer an opportunity to test the 2D capabilities of the numerical models. As the flow in the reservoir will remain subcritical with relatively small-amplitude waves, computations could be checked for excessive numerical dissipation.

5.1.1 Physical experiments

A comprehensive experimental study of a dam-break flow in a channel with a 90 bend has been reported by Frazão and Zech (2002, 1999a, 1999b). The channel is made of a 3.92 and a 2.92 metre long and 0.495 metre wide rectilinear reaches connected at right angle by a 0.495 x 0.495 m square element. The channel slope is equal to zero. A guillotine-type gate connects this L-shaped channel to a 2.44 x 2.39 m (nearly) square reservoir. The reservoir bottom level is 33 cm lower that the channel bed level. At the downstream boundary a chute is placed. See the enclosed figure for details.

Frazão and Zech performed measurements for both dry bed and wet bed condition. Here comparisons are made for the case where the water in the reservoir is initially at rest, with the free surface 20 cm above the channel bed level, i.e. the water depth in the reservoir is 53 cm. The channel bed is initially dry. The Manning coefficients evaluated through steady-state flow experimentation are 0.0095 and 0.0195 $s/m^{1/3}$, respectively, for the bed and the walls of the channel.

The water level was measured at six gauging points. The locations of the gauges are shown in Figure 5.1 and the coordinates are listed in Table 5.1.

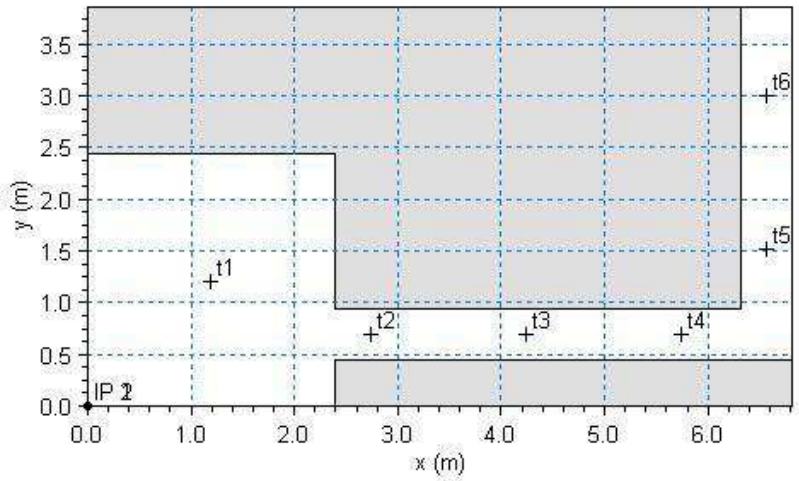

Figure 5.1 Set-up of the experiment by Frazão and Zech (2002)

Table 5.1 Location of the gauging points

Location	x (m)	y (m)
T1	1.19	1.20
T2	2.74	0.69
T3	4.24	0.69
T4	5.74	0.69
T5	6.56	1.51
T6	6.56	3.01

5.1.2 Numerical experiments

Simulations are performed using both the two-dimensional and the three-dimensional shallow water equations.

An unstructured mesh is used containing 18311 triangular elements and 9537 nodes. The minimum edge length is 0.01906 m and the maximum edge length is 0.06125 m. In the 3D simulation 10 layers is used for the vertical discretization. The time step is 0.002 s. At the downstream boundary, a free outfall (absorbing) boundary condition is applied. The wetting depth, flooding depth and drying depth are 0.002 m, 0.001 m and 0.0001 m, respectively.

A constant Manning coefficient of 105.26 $m^{1/3}/s$ is applied in the 2D simulations, while a constant roughness height of $5 \cdot 10^{-5}$ m is applied in the 3D simulation.

5.1.3 Results

In Figure 5.2 time series of calculated surface elevations at the six gauges locations are compared to the measurements. In Figure 5.3 contour plots of the surface elevations are shown at T = 1.6, 3.2 and 4.8 s (two-dimensional simulation).

In Figure 5.4 a vector plot and contour plots of the current speed at a vertical profile along the centre line (from (x,y)=(5.7, 0.69) to (x,y)=(6.4, 0.69)) at T = 6.4 s is shown.

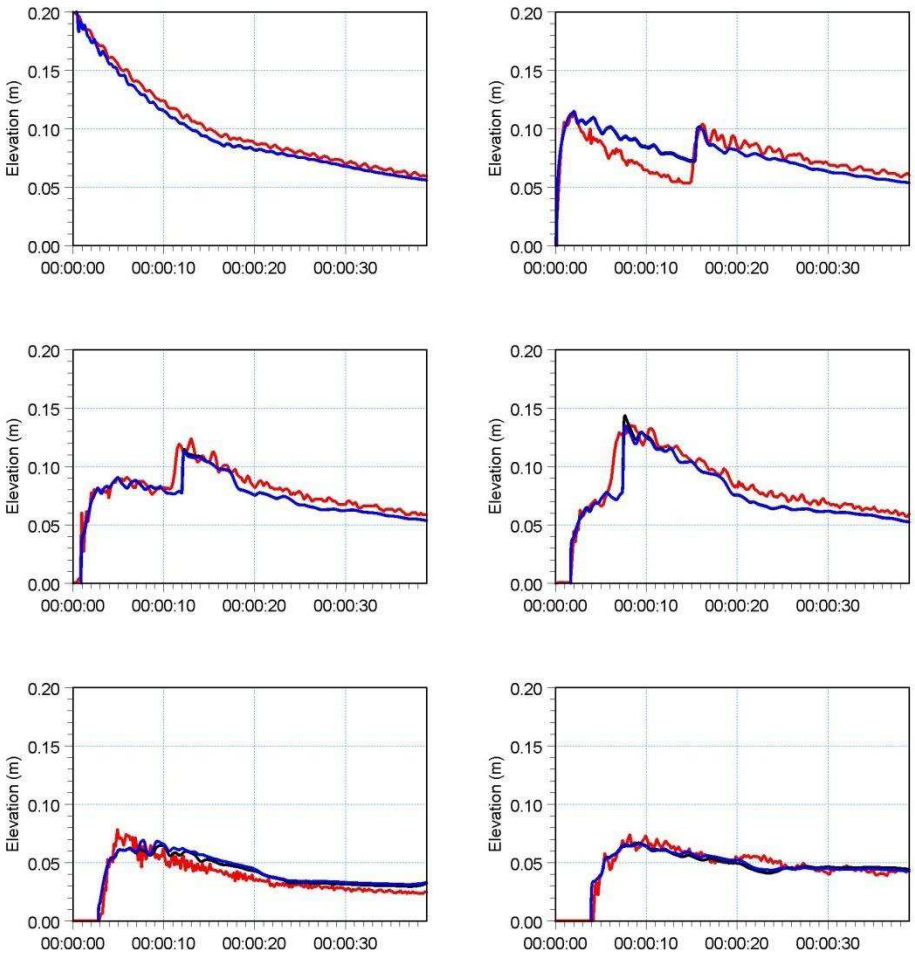

Figure 5.2 Time evolution of the water level at the six gauge locations. (blue) 3D calculation, (black) 2D calculation and (red) Measurements by Frazão and Zech (1999a,b)

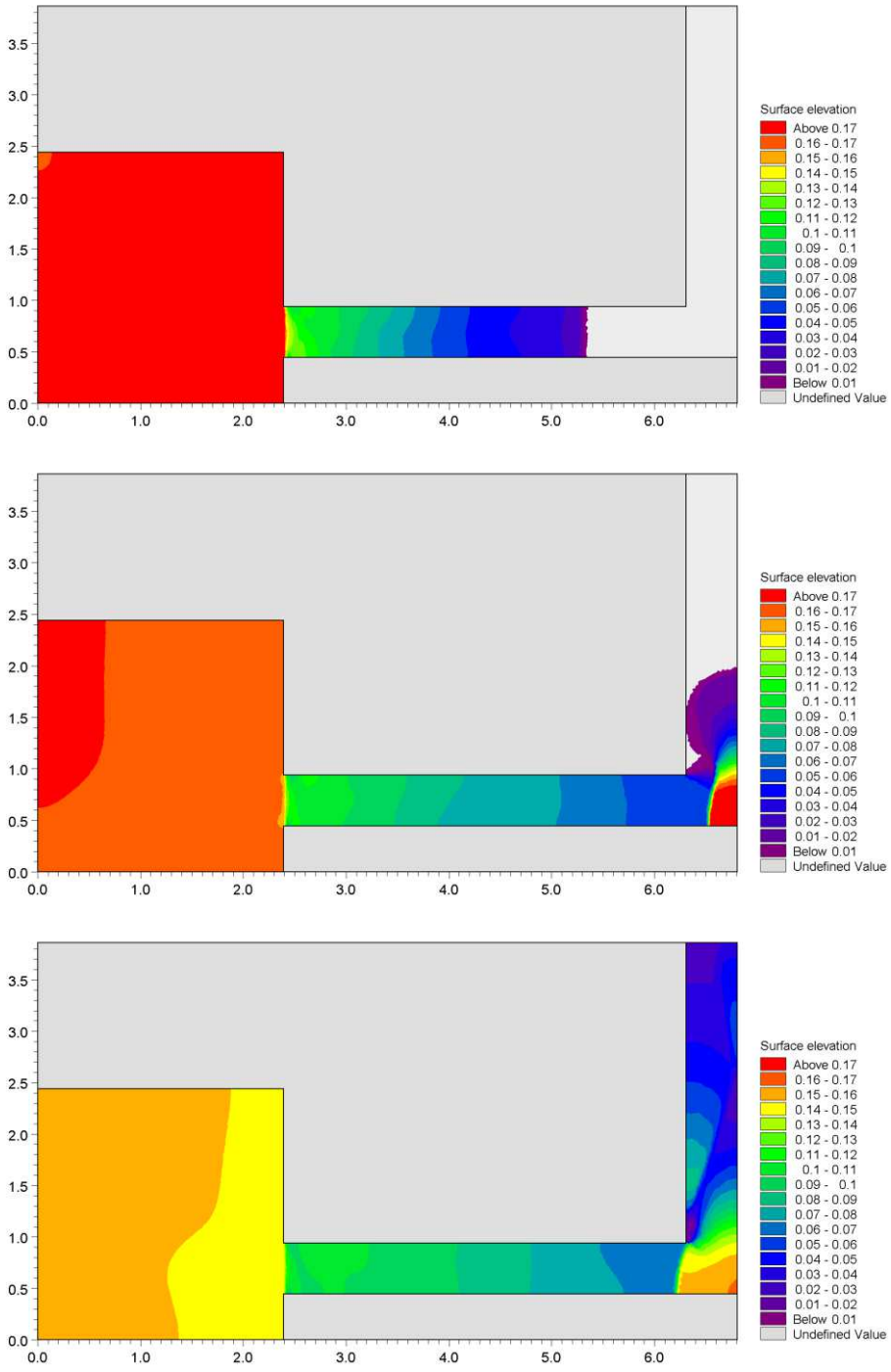

Figure 5.3 Contour plots of the surface elevation at T = 1.6 s (top), T = 3.2 s (middle) and T = 4.8 s (bottom).

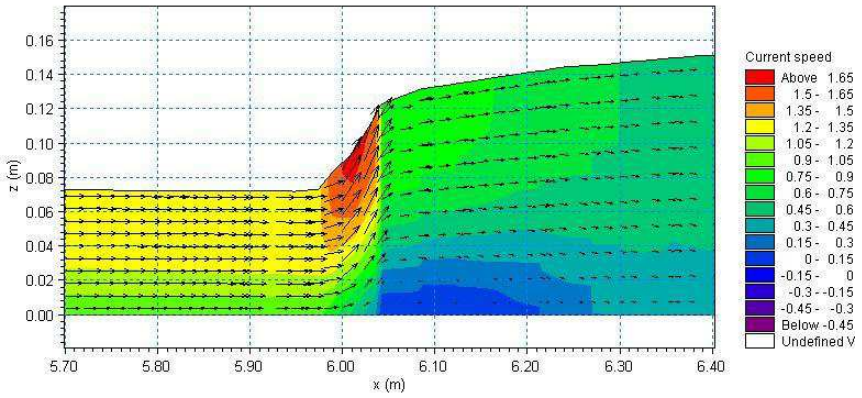

Figure 5.4 Vector plot and contour plots of the current speed at a vertical profile along the centre line at T = 6.4 s

6 References

/1/ Darwish M.S. and Moukalled F. (2003), TVD schemes for unstructured grids, Int. J. of Heat and Mass Transfor, 46, 599-611)

/2/ Fredsøe, J. (1984), Turbulent boundary layers in Combined Wave Current Motion. J. Hydraulic Engineering, ASCE, Vol 110, No. HY8, pp. 1103-1120.

/3/ Geernaert G.L. and Plant W.L (1990), Surface Waves and fluxes, Volume 1 – Current theory, Kluwer Academic Publishers, The Netherlands.

/4/ Hirsch, C. (1990). Numerical Computation of Internal and External Flows, Volume 2: Computational Methods for Inviscid and Viscous Flows, Wiley.

/5/ Iqbal M. (1983). An Introduction to solar Radiation, Academic Press.

/6/ Jawahar P. and H. Kamath. (2000). A high-resolution procedure for Euler and Navier-Stokes computations on unstructured grids, Journal Comp. Physics, 164, 165-203.

/7/ Jones, O., Zyserman, J.A. and Wu, Yushi (2014), Influence of Apparent Roughness on Pipeline Design Conditions under Combined Waves and Current, *Proceedings of the ASME 2014 33rd International Conference on Ocean, Offshore and Arctic Engineering*.

/8/ Kantha and Clayson (2000). Small Scale Processes in Geophysical Fluid flows, International Geophysics Series, Volume 67.

/9/ Lind & Falkenmark (1972), Hydrology: en inledning till vattenressursläran, Studentlitteratur (in Swedish).

/10/ Munk, W., Anderson, E. (1948), Notes on the theory of the thermocline, Journal of Marine Research, 7, 276-295.

/11/ Oddo P. and N. Pinardi (2007), Lateral open boundary conditions for nested limited area models: A scale selective approach, Ocean Modelling 20 (2008) 134-156.

/12/ Pugh, D.T. (1987), Tides, surges and mean sea-level: a handbook for engineers and scientists. Wiley, Chichester, 472pp

/13/ Rodi, W. (1984), Turbulence models and their applications in hydraulics, IAHR, Delft, the Netherlands.

/14/ Rodi, W. (1980), Turbulence Models and Their Application in Hydraulics - A State of the Art Review, Special IAHR Publication.

/15/ Roe, P. L. (1981), Approximate Riemann solvers, parameter vectors, and difference-schemes, Journal of Computational Physics, 43, 357-372.

/16/ Sahlberg J. (1984). A hydrodynamic model for heat contents calculations on lakes at the ice formation date, Document D4: 1984, Swedish council for Building Research.

/17/ Shu C.W. (1997), Essentially Non-Oscillatory and Weighted Essenetially Non-Oscillatory Schemes for Hyperbolic Conservation Laws, NASA/CR-97-206253, ICASE Report No. 97-65, NASA Langley Research Center, pp. 83.

/18/ Sleigh, P.A., Gaskell, P.H., Bersins, M. and Wright, N.G. (1998), An unstructured finite-volume algorithm for predicting flow in rivers and estuaries, Computers & Fluids, Vol. 27, No. 4, 479-508.

/19/ Smagorinsky (1963), J. General Circulation Experiment with the Primitive Equations, Monthly Weather Review, 91, No. 3, pp 99-164.

/20/ Soares Frazão, S. and Zech, Y. (2002), Dam-break in channel with 90° bend, Journal of Hydraulic Engineering, ASCE, 2002, 128, No. 11, 956-968.

/21/ Soares Frazão, S. and Zech, Y. (1999a), Effects of a sharp bend on dam-break flow, Proc., 28th IAHR Congress, Graz, Austria, Technical Univ. Graz, Graz, Austria (CD-Rom).

/22/ Soares Frazão, S. and Zech, Y. (1999b), Dam-break flow through sharp bends – Physical model and 2D Boltzmann model validation, Proc., CADAM Meeting Wallingford, U.K., 2-3 March 1998, European Commission, Brussels, Belgium, 151-169.

/23/ UNESCO (1981), The practical salinity scale 1978 and the international equation of state of seawater 1980, UNESCO technical papers in marine science, 36, 1981.

/24/ Wu, Jin (1994), The sea surface is aerodynamically rough even under light winds, Boundary layer Meteorology, 69, 149-158.

/25/ Wu, Jin (1980), Wind-stress Coefficients over sea surface and near neutral conditions – A revisit, Journal of Physical. Oceanography, 10, 727-740.

/26/ Zhao, D.H., Shen, H.W., Tabios, G.Q., Tan, W.Y. and Lai, J.S. (1994), Finite-volume two-dimensional unsteady-flow model for river basins, Journal of Hydraulic Engineering, ASCE, 1994, 120, No. 7, 863-833.

Principles for distribution of loads

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V1 date		Distributed to:	
Review			
Quality Assurance			

1 Objective

In order to do mechanistic modelling, loads must be allocated to specific positions (grids) in the models and have an associated freshwater source. The methodology for distributing the freshwater is described in /2/ and this note describes the methodology of distributing the nutrient loads.

2 Data used

Load (N & P) data from NST via DCE has been delivered (primo July 2013) and imported in an Access database for further processing.

Furthermore, GIS data for water bodies, catchments (ID15) and streams have been delivered by NST, as well as measured data of nutrients, suspended solids, dry matter etc. within the streams.

repository	folder	File names
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	qp_dogn2579235_5jul13.txt (DCE)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	qn_dogn2579235_5jul13.txt (DCE)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	4.ordens belastninger.accdb (-)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q & load\GIS project\Farvandsområder	Farvandsinddeling.shp (NST)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q & load\GIS project\Belastninger	oplande_id15.shp (NST)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q & load\GIS project\Belastninger	vandlob_vp1.shp (NST)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	Vandkemi_dokumentation.docx (NST)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	Vandkemi1.csv Vandkemi.xls (NST)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	Fordelingsnøgler - uorganiske næringssalte (-)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	kemi.txt (NST)
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q & load\GIS project\Arealanvendelse	Skov.shp (NST)
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\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q & load\GIS project\Arealanvendelse	Vådområder.shp (NST)

Principles for distribution of loads

\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	Stepanauskas_PON.POC.xls
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\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	SSin_pr.mdr_Limfjorden.xls
\\dkcph1-stor.dhi.dk\Projects\11811187-1	Q and loads - Acquired data - DCE	Landuse-relationer_v2.xls

3 General principles

Nutrient load data from Danish catchments to 4th order water body levels has been delivered by DCE. Loads are calculated according to the methodology of the national load calculations but with finer spatial resolution than estimated previously, see /1/, /7/ and Appendix B for methodology.

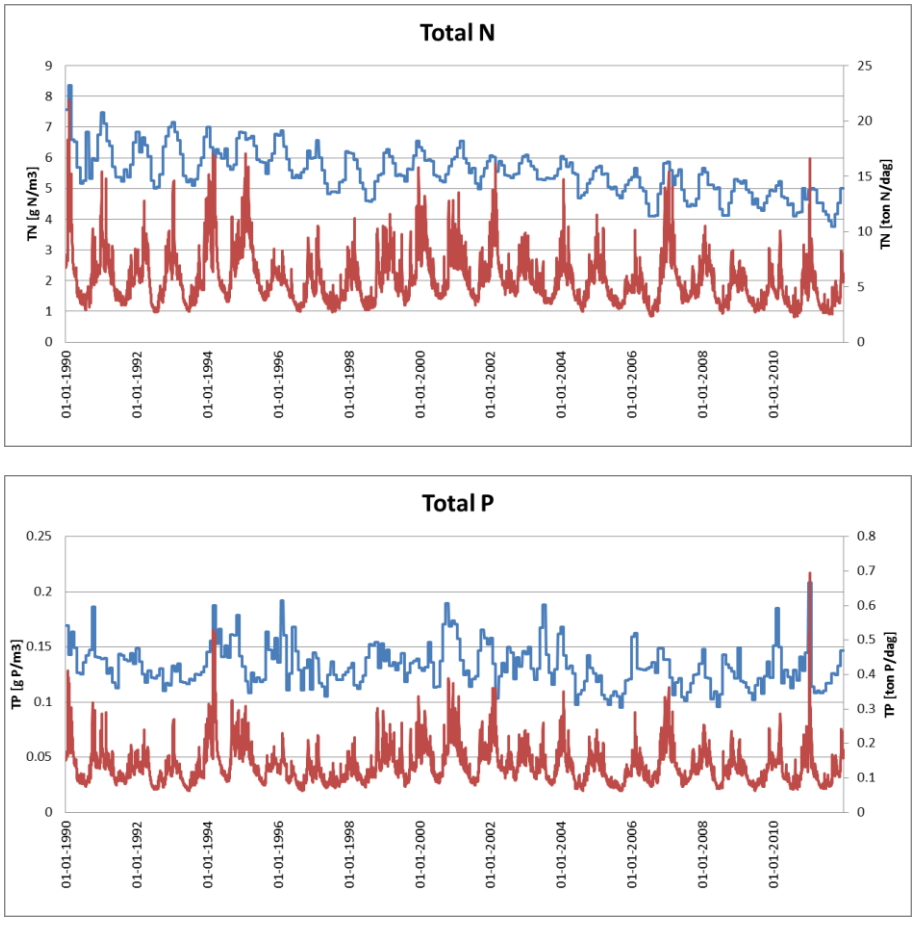


Figure 1: Loading (red line) and concentrations (blue line) of total nitrogen (top figure) and total phosphorus (bottom figure) to Hjarbæk Fjord, 4th order water body no. 3745.

An example of load data for Hjarbæk Fjord (the Limfjord) is shown in **Error! Reference source not found.**. The loads are delivered as a total load per day. The corresponding

Principles for distribution of loads

concentrations of total nitrogen (TN), and total phosphorus (TP) in streams are estimated from total discharge (Q)[1] and total load, see **Error! Reference source not found.**.

A thorough description of monitoring stations and method for estimating the loads can be found in /7/.

In addition to N and P, mechanistic modelling needs information on total organic carbon (TOC) loads and their fractions (dissolved and particulate organic carbon), as well as information on silica loads (Si) and inorganic suspended sediments (SSin). These data are rarely measured and not estimated as part of the national nutrient budgets. Hence, for these loads other strategies has to be implemented, and this note also includes descriptions of methodologies for deriving these parameters.

As freshwater primarily is discharged through stream outfalls, it has been decided in general to allocate almost all loads to these stream outfalls – including direct sewage outfalls and discharge from marine aquacultures. Exceptions are, potentially, the major sewage outfalls (like Lynetten in Copenhagen and Marselisborg in Århus). Such direct loads will be handled as separate sources if evaluated critical to the modelled distribution of nutrients in the recipient.

As described in /2/ the loads are generally ascribed to one single source per 4th order water body and introduced into the models at a location corresponding to the outfall of the largest stream within that water body.

The estimated total daily load of nutrients constitutes the baseline of the nutrient input to the mechanistic marine models. However, the mechanistic marine models developed for this project require nutrient input that is distributed between different species. The different nutrient species simulated (described) by the mechanistic models are listed in Table 1.

Table 1: Pelagic state variables related to nutrients

Name	Comment	Unit
DC	Detritus C	g C m^{-3}
DN	Detritus N	g N m^{-3}
DP	Detritus P	g P m^{-3}
NH4	Total ammonium (NH_4-N + NH_3-N)	g N m^{-3}
NO3	Nitrate+ nitrite, (NO_2-N + NO_3-N)	g N m^{-3}
IP	Dissolved inorganic phosphorous (PO_4-P)	g P m^{-3}
IPss	Inorganic phosphorous (PO_4-P) adsorbed to inorganic sediments	g P m^{-3}
Si	Silicate (SiO_2-Si)	g Si m^{-3}
CDOC	Coloured refractory dissolved organic carbon, DOC	g C m^{-3}
CDON	Coloured refractory dissolved organic nitrogen, DON	g N m^{-3}
CDOP	Coloured refractory dissolved organic phosphorus, DOP	g P m^{-3}
LDOC	Labile DOC	g C m^{-3}
LDON	Labile DON	g N m^{-3}
LDOP	Labile DOP	g P m^{-3}
SSi	Inorganic Solids	g m^{-3}

[1] Distribution of discharge is described in /2/.

Principles for distribution of loads

The methodology for distributing total N and total P into the different N- respectively P-species are described in the following sections, and summarised in Table 2.

Table 2: Overview of strategies for fractionation of TN and TP into inorganic and organic species required by the marine model (see Table 1)

State variable	Measurements (Not measured)	Note
Detritus C	(NM)	Estimated and scaled to detritus N
Detritus N	(NM)	Estimated (from LOI and DC:DN) and scaled to TN
Detritus P	(NM)	Estimated (from LOI and DC:DP) and scaled to TP
Detritus Si	(NM)	Not assumed to be an important part of Total Si loadings, and hence neglected.
NH_4	NH_4	Estimated based on monthly relationships between measured NH_4-N and TN in the stream, see section 0.
NOx (NO_2+NO_3)	NOx	Estimations based on monthly relationships between measured NOx-N and TN in the stream, see section 0.
PO_4	PO_4	Estimations based on monthly relationships between measured PO_4-P and TP in the stream, see section 0.
IPss	(NM)	Can be significant for phosphor transport to the coast. Especially in connection to heavy rain. This parameter has not been measured.
SiO_2	SiO_2	Concentration time series constructed from sporadic measurement as part of NOVA/NOVANA, see section **Error! Reference source not found.**.
CDOC	0.80 × DOC	Literature
CDON	0.69 × DON	Literature
CDOP	0.25 × DOP	Literature
LDOC	0.20 × DOC	Literature
LDON	0.31 × DON	Literature
LDOP	0.75 × DOP	Literature
SSi	0	Can be important for light attenuation. For some model relations to Q has been applied whereas other models does not include SSi.

Principles for distribution of loads

Principles for distribution of loads

4 Determining the dissolved inorganic fractions of TN and TP

In order to determine the dissolved inorganic fraction of the total N and P loads, monitoring data from a number of stations in the “measured catchments” have been analysed as basis for the distribution. As guidance[2], only stations with extended time series are included, see /7/ for details on monitoring stations included.

The analyses of the fraction of dissolved inorganic nutrients are made per 4th order water body, as is the resolution of the load data, and thus each monitoring station has been associated with a catchment of a 4th order water body. The links between monitoring stations, the stream they are located in and the associated 4th order water bodies are listed in Appendix A. Figure 2 illustrates some of the monitoring stations included in the load estimation, with focus on the catchments of the Limfjord.

The breakdown of TN and TP into inorganic and organic nutrients is exemplified by the analysis of the Limfjord.

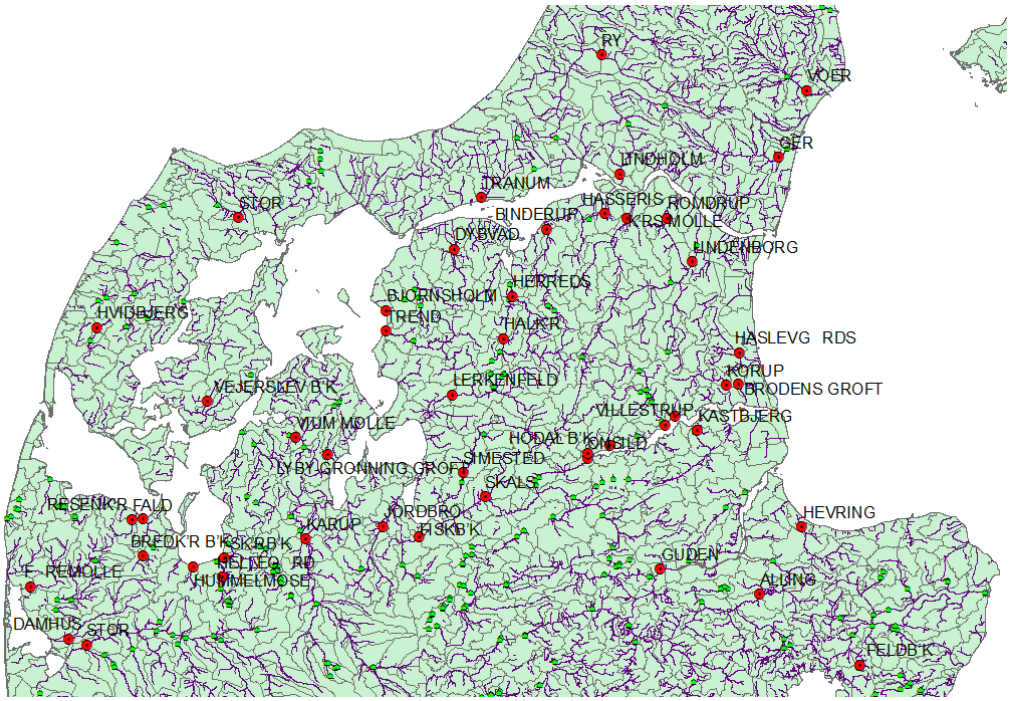


Figure 2: Example of all NOVANA monitoring stations (green dots) and the monitoring stations (red dots) applied for the load calculations reported in /1/ and /7/.

[2] For the main part of monitoring stations in streams discharging to Limfjorden (see red dots in Figure 2) data has been collected frequently and since the beginning of the 1990’ties with one to two water quality samples collected every month. The stations selected for the analyses have over the last approximately 20 years 20 or more datasets of corresponding measurements of total N and inorganic N and similar with P. For other water bodies sampling may be less complete – this will show when we start to analyse these data and we may have to compromise.

Principles for distribution of loads

4.1 Determining the inorganic fractions (NO_x and NH_4) of TN

For the main part of monitoring stations shown in red dots in Figure 2, data has been collected frequently since the beginning of the 1990'ties. These monitored data are used to determine the inorganic fractions (NO_x and NH_4) of TN, as described below and in Figure 3.

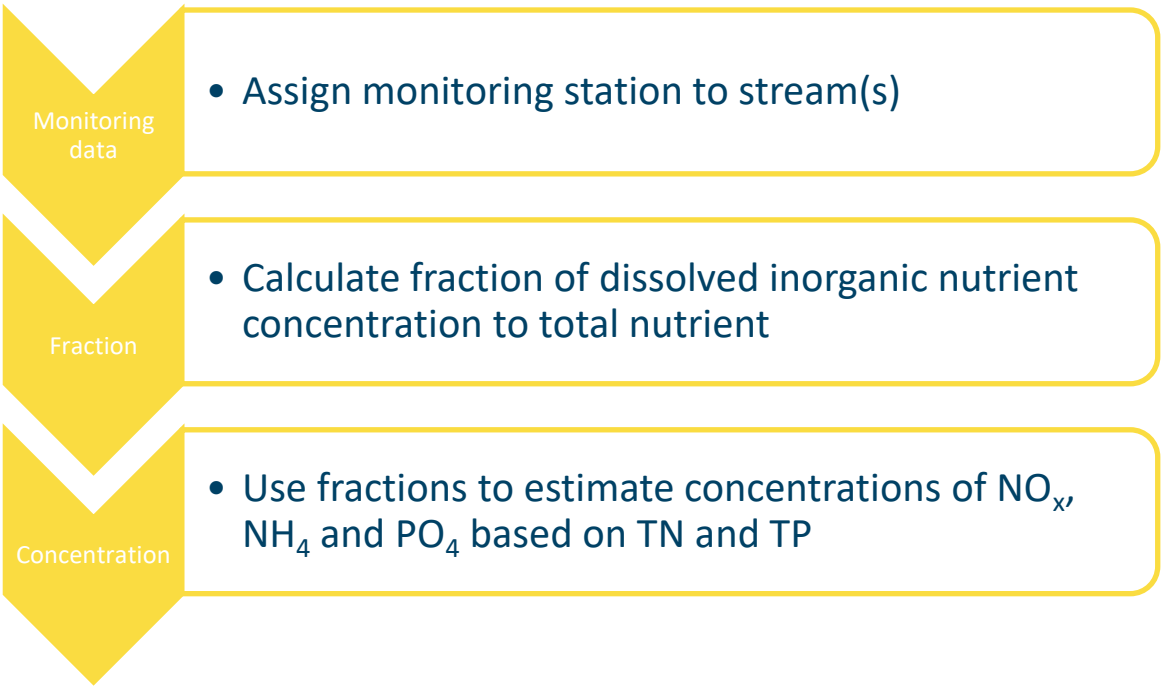


Figure 3: Schematic figure of the method for determining the dissolved inorganic fractions nutrients of total nutrients.

At first, each monitoring station is assigned to one or more streams within the vicinity of the location of the monitoring. Only downstream stations are used. Obviously the stream where the monitoring stations is located is included, and e.g. in the model four streams are included for Hjarbæk fjord, and they all have one unique monitoring station assigned, see Appendix A for more details.

At Mors, on the other hand, only one monitoring stations exists, why this stations is assigned to all streams on Mors and hence represents inorganic fractions (NO_x and NH_4) of TN for streams from Mors to the 4th order water bodies: Agerø Bredning/Nees Sund and Visby Bredning/ Vilsund. Likewise, all monitoring stations within the Limfjord catchment have been assigned to stream outlets to the Limfjord, and the method is applied for all other mechanistic models.

For each sampling occasion (usually monthly intervals), the fractions of NH_4-N to TN, and NO_x-N to TN has been estimated for each monitoring station. In case that the sum of inorganic N fractions is larger than the measured TN, the data set has been discarded. Based on the estimated fractions per date, monthly means (averaged over 20 years) and StDev's are calculated.

Figure 4 shows an example of the yearly variation in the NOx-fraction from a monitoring station located in the catchment to Hjarbæk Fjord (4th order water body no. 3745). Furthermore, ± StDev is included to illustrate variation between the years of monitoring. For this station the nitrate fraction constitute about 90% ± 10-15% SD of total nitrogen

Principles for distribution of loads

with minor seasonal variation. Figure 5 shows the fractions of inorganic N to TN and the shares by NH_4 and NO_x for all 4 streams discharging in the model to the 4th order water body 3745, Hjarbæk Ford. The fraction of DIN is about 80-90% whith NO_x majorly dominating. At 3 of the 4 stations there is a tendency to a little higher share of NOx in late spring-early summer and a lower share in late summer- autumn. Table xx in section **Error! Reference source not found.** gives the statistics for all 4th order water bodies and here the overall patterns are also discussed.

This method is carried out and applied for each monitoring station included in this study and associated loadings on a 4th order water body level.

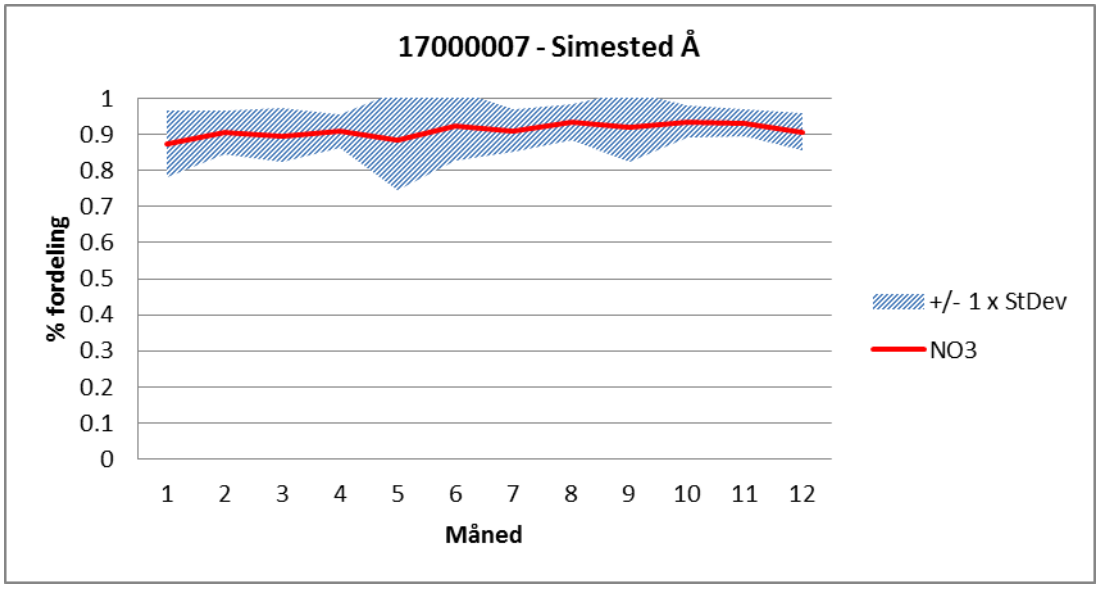
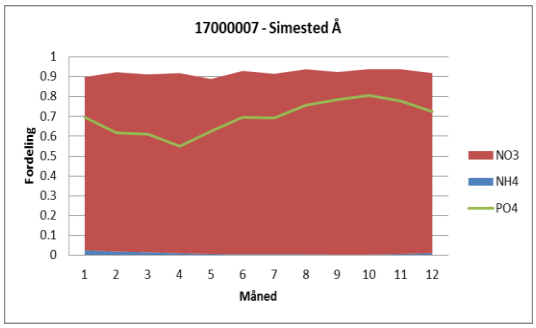
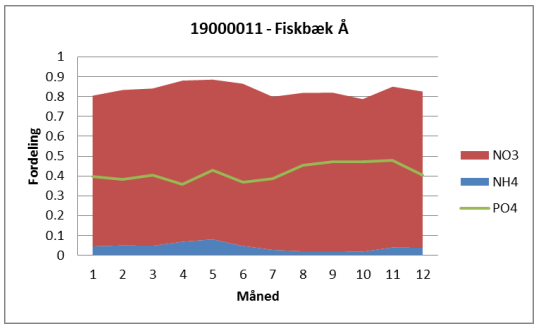


Figure 4: Annual variation in monthly means of the fraction of NO_x-N to TN, including ± 1 StDev for an upstream monitoring station (17000007) in Simested Å discharging to 4th order water body 3745, Hjarbæk Fjord. Data covers 20 years with ca. 24 sampling per year. Data sets where the fraction of DIN exceeded 100% have been omitted from the following analysis.





Principles for distribution of loads

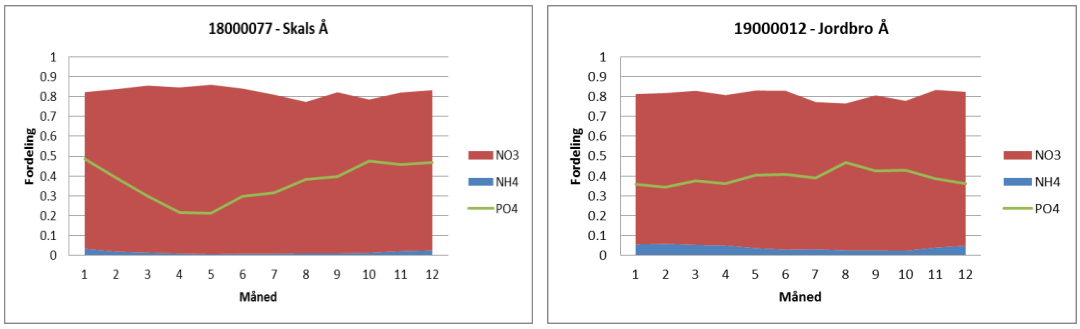


Figure 5: Annual variation in the fraction of inorganic N and P. Also showing the distribution of inorganic N between NH_4-N (blue area), and NO_x-N (red area). The stream and monitoring stations all associate with Hjarbæk Fjord, 4th order water body no. 3745.

4.2 Determining the inorganic P fraction of total P

A similar approach as for nitrogen has been applied to estimate the fraction of phosphate (DIP) to total P. Based on data from the same stream monitoring stations monthly data sets are compiled and the monthly means and StDev's has been calculated.

The results of the calculation for the station in Simested Å discharging to Hjarbæk Fjord (4th order water body 3745), Limfjorden, are shown in Figure 6. Compared to DIN the fraction of DIP is generally lower and with more seasonal variation. Some differences are observed between the stations. Figure 5 shows the mean of the 4 monitoring stations in the catchment of Hjarbæk Fjord. In Fiskebæk Å the fraction of DIP is lowest, constituting about 40% of TP. The highest fraction is measured in Simested Å, up to 80% during autumn. All stations showed an increase in late summer-autumn but only Simested and Skals Å showed pronounced seasonal variation with noticeable decrease in late spring-early summer (around April) and increase in autumn. .

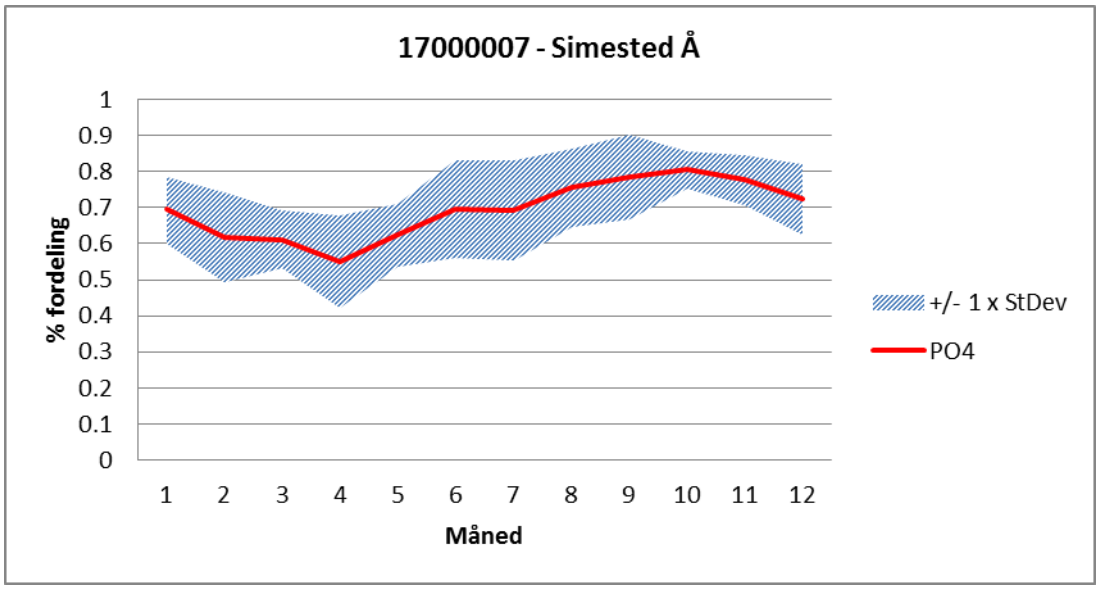


Figure 6: Annual variation in monthly means of the fraction of PO_4-P (DIP) to TP, including ± 1 StDev for an upstream monitoring station (17000007) in

Principles for distribution of loads

Simested Å discharging to 4th order water body 3745, Hjarbæk Fjord. Data covers 20 years with ca. 24 sampling per year..

4.3 Uncertainties

Some uncertainties do of course exist as we do not have measurements from all streams included in the model. Using Figure 2 as an example it is obvious that the water quality monitoring stations does not represent all streams and catchments and for some areas only few stations are included.

As the inorganic nutrient fraction versus the organic fraction depends on soil type, land use etc. any variations occurring within catchments are not accounted for in the applied approach.

4.3.1 Inorganic nutrients versus total nutrients

We have chosen to include measurements over the past 20 years (if available) when evaluating the fraction of inorganic nutrients versus total nutrients to have a larger amount of monthly data to support the seasonal distribution. However, land use and agricultural practice has changed over the last 20 year which might have influenced the relation between inorganic nutrients and total nutrients.

4.3.2 Retention downstream observations

The estimated loads is based on measurements taken somehow upstream in the respectively rivers. From the measurement station to the marine waters some N retention is taken place, a retention that is estimated in the load calculations, see /7/. However, that down-stream retention has not verified and is uncertain.

4.3.3 Inorganic P

In contrast to nitrogen, a larger part of phosphorous is known to be transported in pulses as PO_4 adsorbed to inorganic suspended particles, bound in organic particles and partly as bed-load. Therefore, load estimates based on weekly or bi-weekly water samples of total P inherently will be uncertain and most likely will underestimate the total P load (because bed-load transport will not be represented in water samples). In the loads provided by DCE the P load from monitored catchments are based on single samples whereas the P load from non-monitored catchments includes some estimates from small catchments based on continuous measurements. Hence, the P loads from non-monitored catchments are generally larger than from monitored catchments, and we expect the P load from monitored catchments to be underestimated.

If we during modelling discover a miss-match between the P load and the P concentrations in the recipient, we might need to address this by introducing of some relationship between discharge and land-use (agricultural area or forest areas dominating) or the amount of downstream lakes within the catchment in question.

Principles for distribution of loads

5 Organic matter and nutrients

Where section **Error! Reference source not found.** handles the method for separating dissolved inorganic N and P this section handles the remaining part: The organic fraction of TN respectively TP as well as the organic carbon fraction. The overall method is schematically described in Figure 7 and during the follow sections

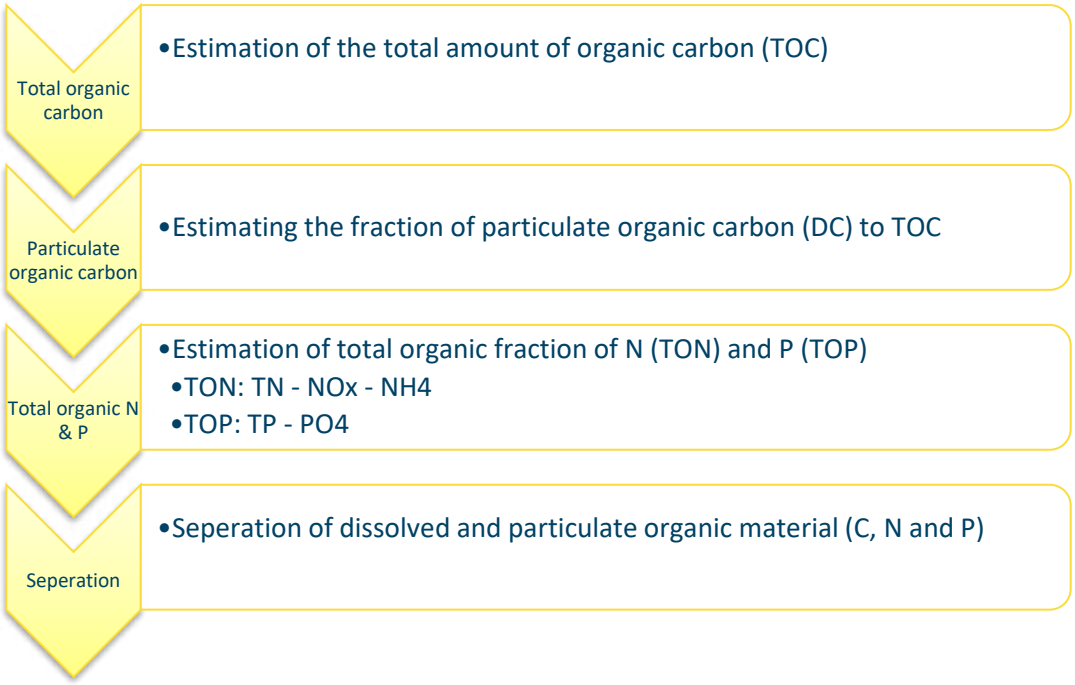


Figure 7: Schematic figure of the method for determining the organic fractions of the total nutrients.

5.1 Total organic N and P

The fraction of total N bound in organic material is estimated as the total N minus inorganic N (NH_4 + NO_x), see section 4.1. Organic bound nitrogen can exist in a particulate fraction (detritus N, DN) and in a dissolved fraction (DON). Unfortunately, these fractions are not measured but must be estimated indirectly from the corresponding concentrations of particulate organic carbon, i.e. detritus C (DC) and dissolved organic carbon (DOC).

Phosphorus and its speciation are more complicated because the particulate fraction can include both inorganic P and organic P. Initially, we will estimate the “unreactive” (organic) P fraction as the difference between TP and PO_4 but most likely we will refine this issue in more details when modelling commence.

5.2 Organic carbon

The data collected under the national monitoring program NOVA/NOVANA include a limited number of measurements of organic carbon and other data that can be converted

Principles for distribution of loads

to organic carbon. The measurements relevant to this modelling exercise are listed in Table 3.

Because of the limited number of measurements (Table 3) it is not possible to estimate both fractions (DC and DOC) on a temporal (monthly) and on a spatial (catchment) scale.

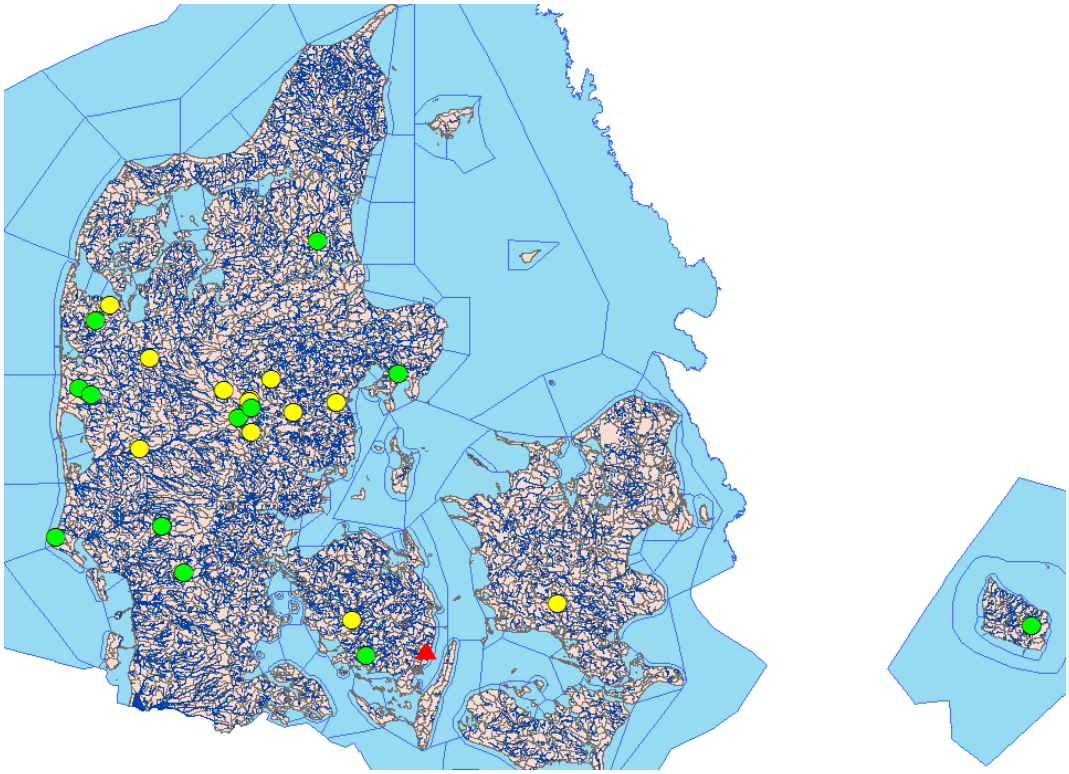


Figure 8: Location of applied monitoring stations for estimations of DC/TOC. Markings represents monitoring stations with TOC (red triangles (notice the figure includes two stations very close, why this is not visible)), NVOC (green dots) and COD (yellow dots) measurements.

Both TOC and NVOC are direct measurements of total organic carbon, and hence, can be used directly. However, TOC and NVOC measurements are few and sporadic and time series cannot be constructed for neither of the two measurements. Hence, for TOC and NVOC estimations are lumped without analysing locations, seasons nor years of the measurements. The number of samples shown in Table 3 indicates the total amount of measurement from ODA, however, to be used for this analysis we seek sets of data where both LOI and one of the three other measurements (TOC, NVOC or COD) exists. This procedure reduces the amount of measurements dramatically, see Table 5.

As a supplement total Chemical Oxygen Demand (COD) is applied as an indirect measurement of TOC. A larger amount of data exist for COD, and few monthly mean time series have been constructed where sets of COD and LOI exists, see Figure 8 and Figure 9.

Principles for distribution of loads

Table 3: Number of samples where organic carbon or indicators of organic carbon has been measured in streams.

Organic carbon or indicators of organic carbon	Number of samples
Chemical Oxygen demand (COD) (Total)	21270
Total Organic Carbon (TOC)	757
Non Volatile Organic Carbon (NVOC)	2057
Loss on Ignition (Suspended solids)	29213

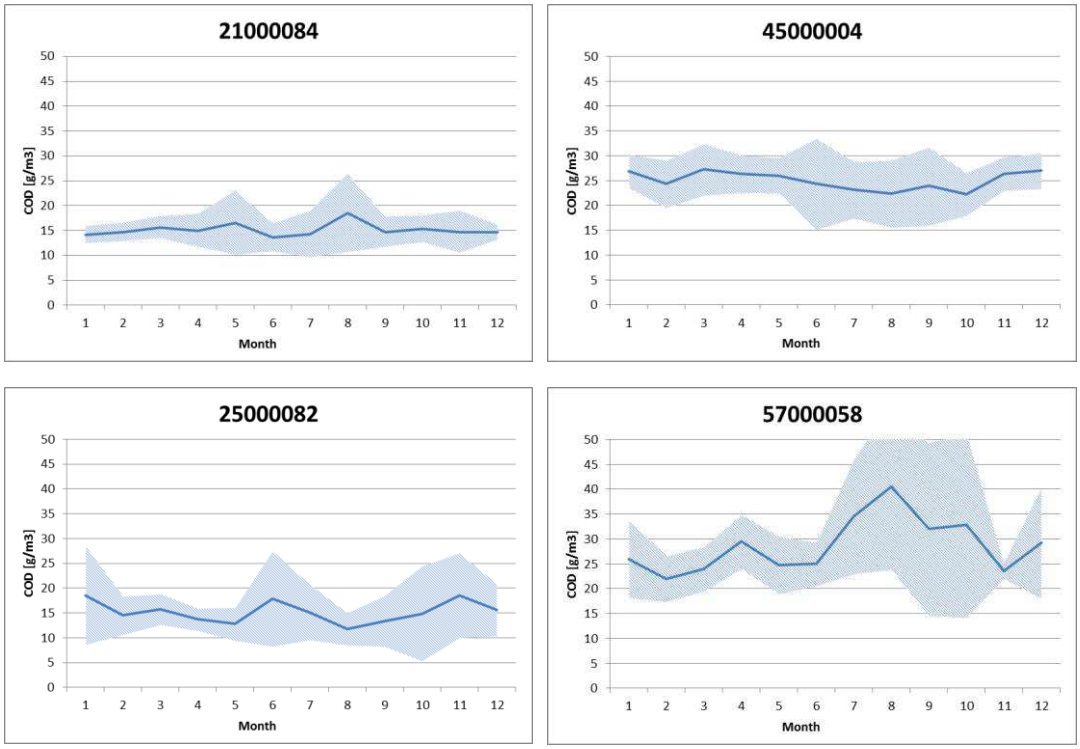


Figure 9: Time series of COD at four different monitoring stations, see Figure 8 for locations. Solid line is average concentrations and shaded area illustrates ± 1×StDev.

In Figure 9 time series of COD is shown and in Table 4 average conversion factors to estimate organic carbon from COD and from LOI are listed.

Table 4: Figures for converting COD and LOI to organic carbon.

Variables	Value	Reference
Total organic carbon (dissolved & particulate) to COD	0.28 g C/g O	
Particulate organic carbon to LOI	0.30 g C/g LOI (range 0.2-0.37)	

Principles for distribution of loads

We assume that Loss on Ignition (LOI) is an accurate measurement of organic content in suspended solids. Hence, LOI is used to estimate the fraction of particulate carbon content, corresponding to the fraction of detritus C (see Table 1).

As for COD, time series of LOI are constructed, see Figure 10, and converted to particulate organic carbon using Table 4. Finally, the fraction of DC to TOC is estimated, see Figure 11.

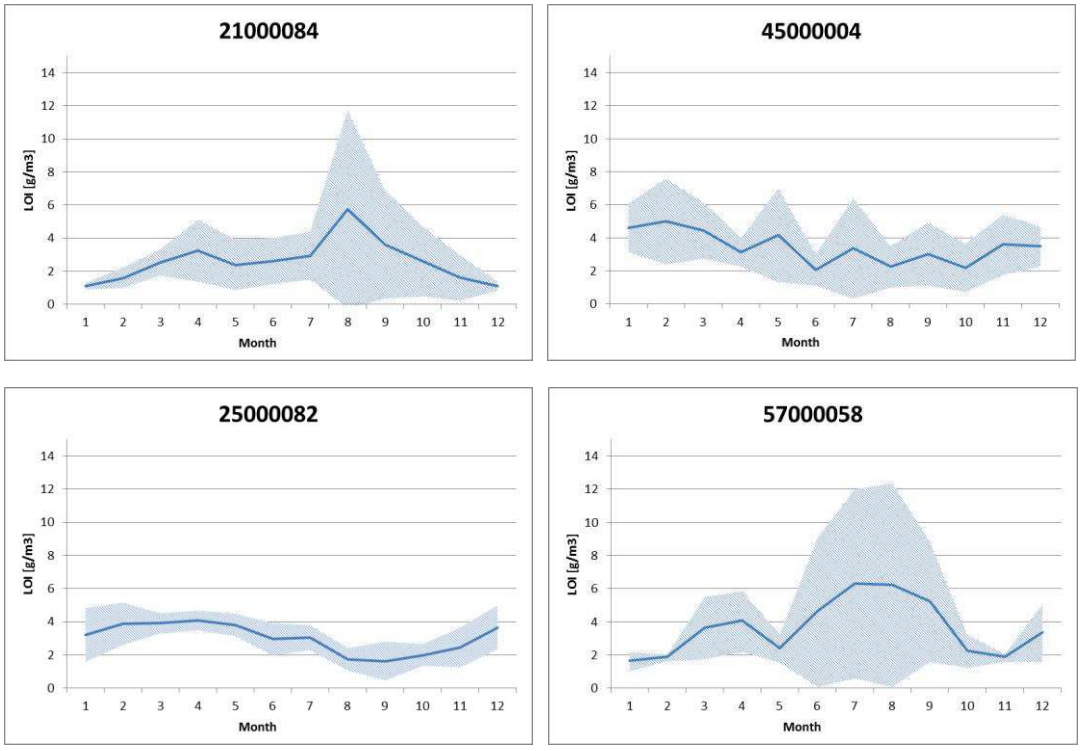
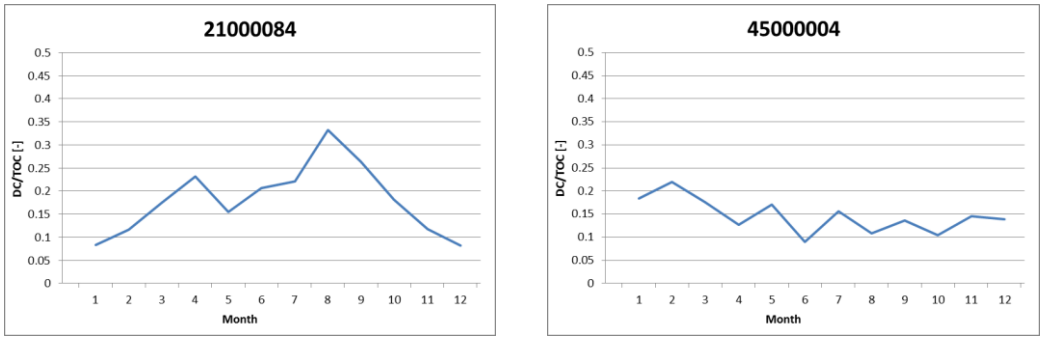


Figure 10: Time series of LOI at four different monitoring stations, see Figure 8 for locations. Solid line is average concentrations and shaded area illustrates ± 1×StDev.



Principles for distribution of loads

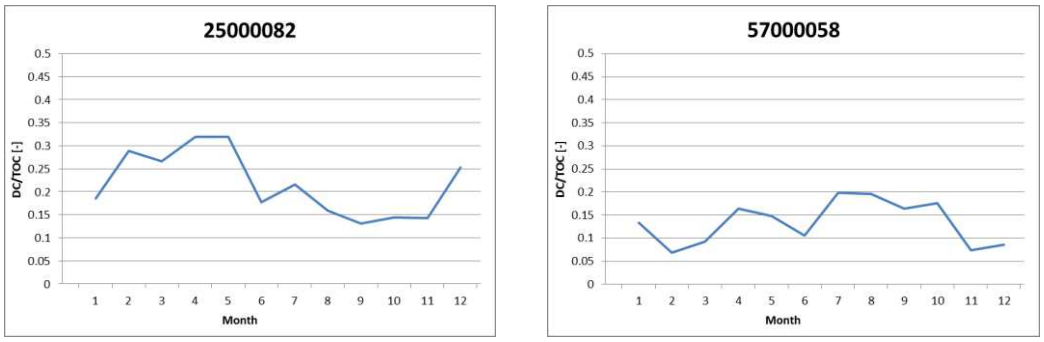


Figure 11: Time series of the DC to TOC fraction at four different monitoring stations, see Figure 8 for locations.

As can be seen from Figure 11 differences in time and between locations exists, but with no clear seasonal patterns and with only few stations to support regional/local patterns all measurements are used to estimate one lumped fraction of DC to TOC. Hence, COD as well as TOC and NVOC are used to estimate one fraction, see Table 5.

In Table 5 the StDev is comparable to the average values indicating some variation not accounted for in this relatively simple method. However, as the fraction of organic to total nutrients is low, as seen in section 0, and as we have only limited amount of measurements to ensure a uniform and repeatable method on a nationwide scale and for later scenarios, the lumped value of 28% in Table 5 is adopted for estimating the fraction of DC to TOC.

Table 5: Fraction of DC to TOC based on different direct or indirect measurements of TOC.

TOC origin[3]	Average	StDev	n
DC/TOC	0.21	0.25	128
DC/NVOC	0.21	0.22	167
DC/COD	0.29	0.23	342
DC/ Avr. (TOC, NVOC & COD)	0.23	0.23	637

5.3 Organic nitrogen and phosphorous

To estimate detritus N (DN, i.e. particulate organic nitrogen), dissolved organic N (DON), detritus P (DP) and dissolved organic P (DOP) we will assume C:N:P ratios for both detritus as well as dissolved organic matter. The ratios applied primarily came from an extensive USGS data set encompassing 28400 water samples (from ca. 500 streams each sampled between 6 and 1440 times during the period 1991-1997) analysed for organic carbon and nutrients (dissolved, particulate, inorganic, organic) along with basic hydrological parameters such as discharge. Prior to analysis stream data were selected to “match” (represent) Danish conditions, i.e. data with high ammonia (> 3 µm NH4-N) indicating sewer discharge were eliminated and only data with seasonal NOx peaks

[3] All estimates of detritus C (DC) are based on LOI measurements.

Principles for distribution of loads

between 0.8 and 10 µM were included. Monthly averages of nutrient concentrations and ratios were estimated for each stream, analysed for seasonal variation and the yearly averages (C:N:P ratios) were plotted against Q to examine if size of water course affected the ratios. Data used for this study is listed in Table 6

Table 6: C:N:P ratios for detritus respectively dissolved organic matter.

Variables	C:N:P [g C:g N:g P]	Reference
Detritus	DCx:DNx:DPx 32:5.5:1	Appendix B
Dissolved organic matter	DOCx:DONx:DOPx 625:41:1	Appendix B

Based on the values in Table 6 and the following equations the relation between DN and DON respectively DP and DOP are estimated. In the following, the relations are solved for N as example, but same procedure is applicable for P. We know that

$$TOC = DC + DOC \; and \; TON = DN + DON$$

where TOC is total organic C, DC is detritus C, DOC is dissolved organic C, TON is total organic N, DN is detritus N and DON is dissolved organic N. Also, we know that

$$DC = DN \times \frac{DCx}{DNx} \; and \; DOC = DON \times \frac{DOCx}{DONx}$$

Where DCx, DNx, DOCx and DONx are from Table 6.

Finally, from section 5.2 we estimated that

$$DC = 0.23 \times TOC \; and \; DOC = 0.77 \times TOC$$

Solving these sets of equations allow us to estimate the different fractions, see Table 7.

Table 7: Fraction of particulate organic nutrients (DN and DP) and dissolved organic nutrients (DON and DOP)

Nitrogen		Phosphorous		Carbon	
DN	DON	DP	DOP	DC	DOC
0.44 × ON	0.56 × ON	0.85 × OP	0.15 × OP	DN×5.8	DON×15.2

5.4 CDOM versus LDOM

Based upon /6/ the fraction distribution of CDOM and LDOM has been adopted, see Table 8. Table 8 also includes estimated fractions of particulate nutrients to dissolved nutrients. These fractions are different compared to Table 7, but land-use is also different between Danish land-use and Baltic country land-use. We still apply the estimated

Principles for distribution of loads

relation between labile dissolved organics and coloured dissolved organics, as described in Table 8.

Table 8: Distribution between particulate and dissolved organic material and splitting of the dissolved organics into labile dissolved organics and coloured dissolved organics. Estimations based on /6/.

Organic P			
DP	66.7%		
DOP	33.3%	LDOP	75%
		CDOP	25%
Organic N			
DN	21.2%		
DON	78.8%	LDON	31%
		CDON	69%
Organic C			
DC	=TOC-DOC		
DOC		LDOC	20%
		CDOC	80%

6 Concentrations of Silicate

Silicate (SiO_2-Si) is also an important nutrient to some primary producers like diatoms and in the open waters silicate can be a limiting nutrient to the pelagic algae in some periods (spring bloom). Hence, Silicate is a part of the mechanistic models setup for the North Sea as well as the inner Danish waters (including the Baltic Sea), why we need to estimate realistic concentrations of inorganic silicate for the models applied for this study, where diatoms as single species is included.

In contrast to N and P loads of silicate is not calculated on a nationwide scale why the same approach as for N and P (see section **Error! Reference source not found.**) is not applicable.

Principles for distribution of loads

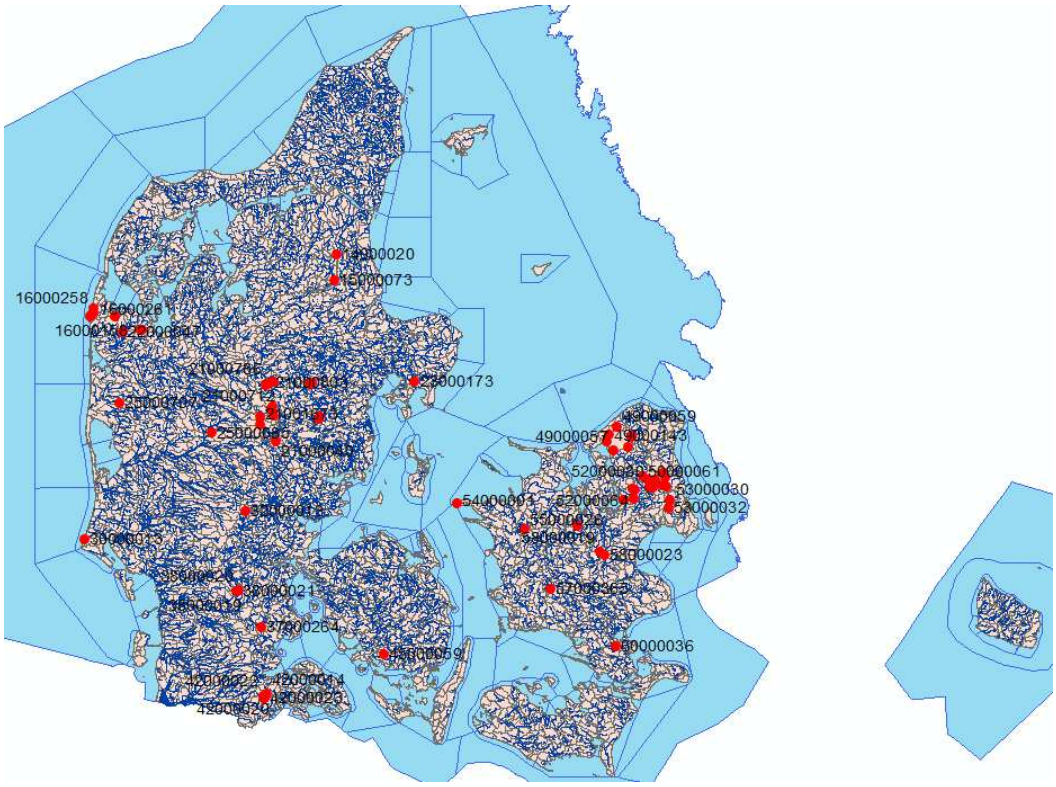
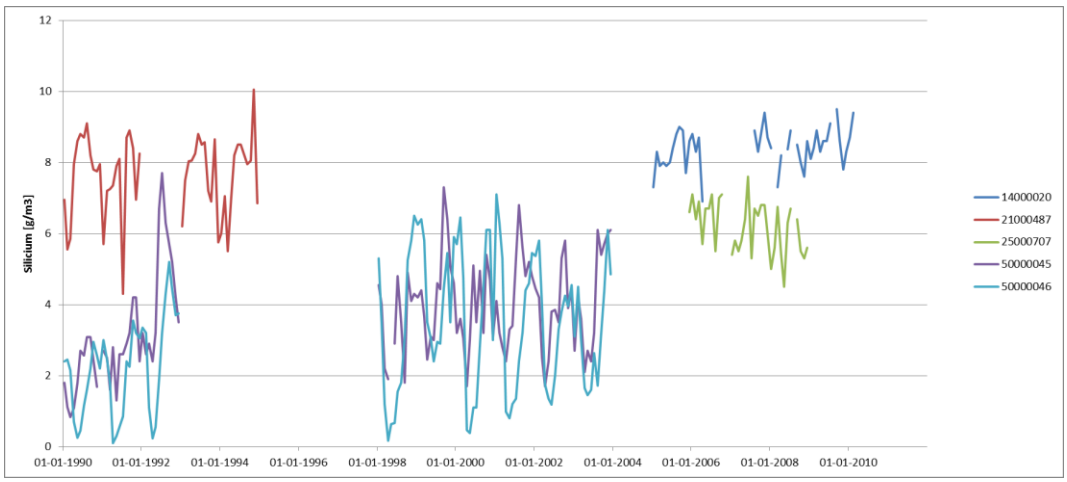


Figure 12: Illustration of monitoring stations with more than 20 measurements of Si from the period 1999-2012. These monitoring stations have been used to estimate the Si concentrations for all associated 4th order water bodies.

From ODA reported concentrations of silicate, where the monitoring stations include more than 20 measurement over the period from 1990-2012, has been identified, see Figure 12. The coverage and continuity of the measurements varies significantly over the stations included in Figure 12. However, the differences in concentrations seems to be somehow related to regions and from the few long-term time series identified there seems not to be an development in time, see Figure 13.

From Figure 13 it might be argued that some development does occur in the early 1990'ties but we do not find any evidence for this – nor explanation – and from the period of the modeling (year 2002 and forward) there are no clear trends, except for some seasonal variation.



Principles for distribution of loads

Figure 13: Time series of Si measurements from 5 different monitoring stations (Source: ODA)

For each of the stations included in Figure 12 monthly averaged concentrations are constructed, see Figure 14. These constructed time series are then appointed a number of streams for each 4th order water body in the inner Danish waters as well as for the North Sea, according to the stream described in /2/.

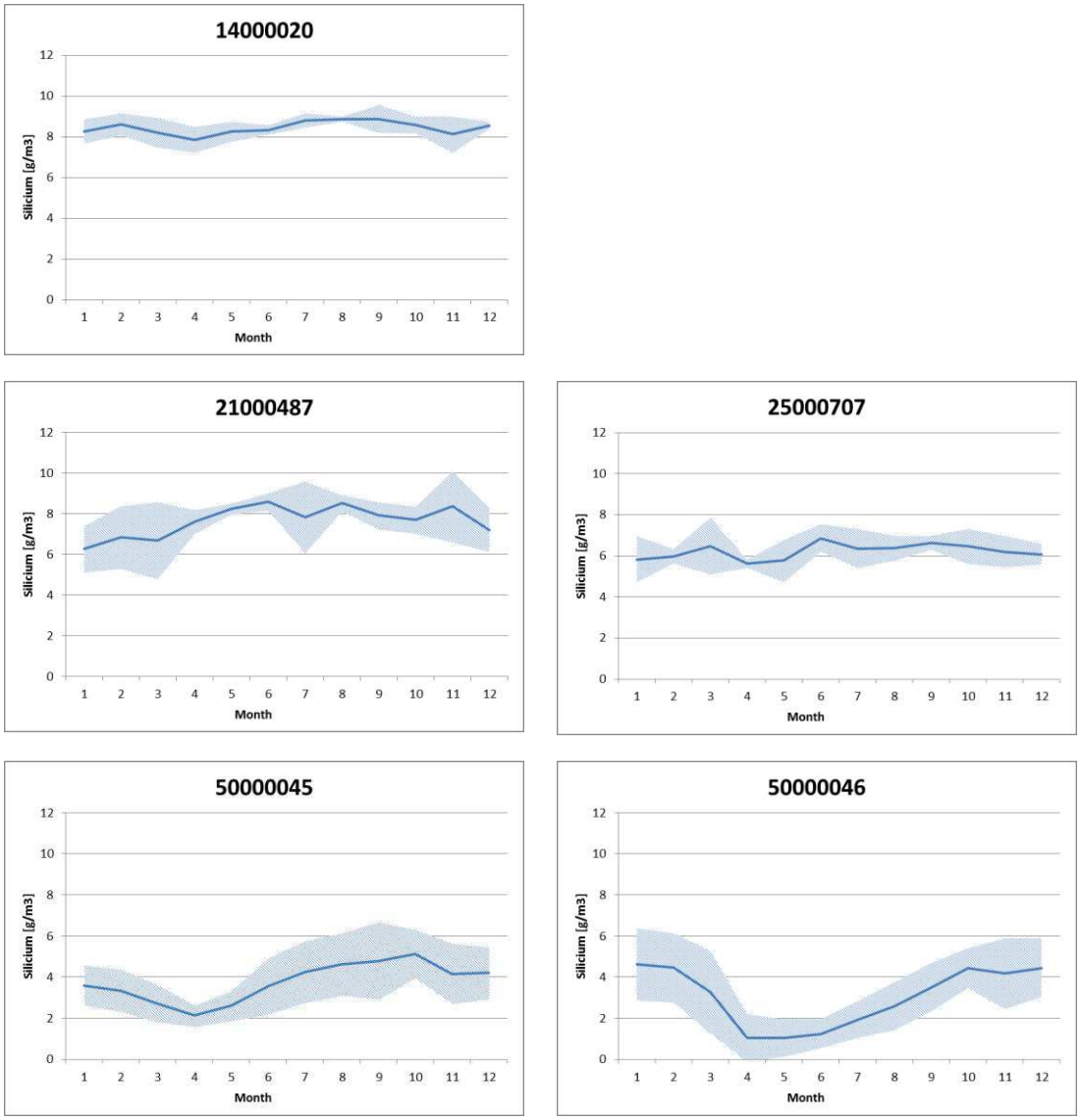


Figure 14: Monthly averages ± 1×StDev of Si at 5 different monitoring stations, see Figure 13.

The monitoring stations included in Figure 14 are located in Jutland (14000020, 21000487 and 21000707 and Zealand (50000045 and 50000046) and as can be seen the three stations in Jutland has concentrations between 6-9 g SiO_2-Si/m^3 with only little or no seasonality whereas the concentrations in Zealand is between 1-5 g SiO_2-Si/m^3 but with more pronounced seasonality.

The variability expressed as ± StDev is more or less to constant 1 g SiO_2-Si/m^3.

Principles for distribution of loads

As for N and P each monitoring stations identified having sufficient amount of data will be appointed a number of streams corresponding to the area of the different monitoring stations, see Appendix A for details.

7 Inorganic Solids

As a final component in (some of) the mechanistic models inorganic solids (SSin) has to be included. SSin is an important parameter as the concentration of SSin has an impact on the light attenuation in the receiving waters (4th order water body). Furthermore, SSin is known to be potential important for transport of adsorbed inorganic P (IPss) as mentioned in section **Error! Reference source not found.**.

Concentrations of SSin have previously been described as a function of discharge /8/ and for this study we adopt this concept for monitoring stations where relations can be developed.

In the stations shown in Figure 15 sets of data on both suspended solids (SS) and loss on ignition (LoI) exists, and hence, by subtracting SS with LoI the amount of inorganic suspended solids (SSin) can be estimated. In the following these data are used to estimate relations between daily discharge (as delivered by DCE and described in /2/) and estimations of SSin (SS-LoI).

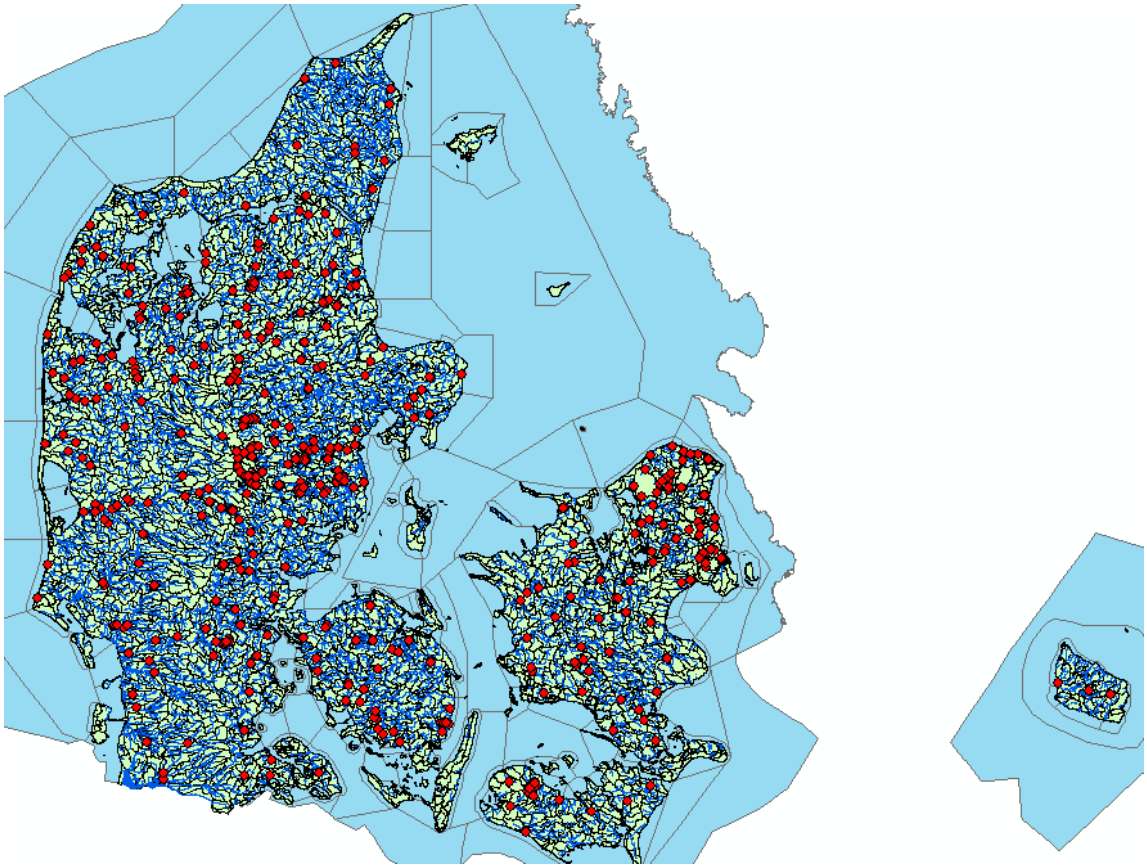


Figure 15: Illustration of monitoring stations where measurements of inorganic suspended solids (SSin) exists. Downstream stations have been used to estimate relations between SSin and discharge.

Principles for distribution of loads

As described in previous sections each monitoring stations is appointed to a number of streams to cover all 4th order water bodies depending on locations of monitoring stations and streams included in the modelling, see /2/.

However, these relations cannot be transformed directly from one catchment to another before some uniformity has been adopted. To obtain uniformity we build the relations to discharge by calculating discharge divided by catchments area: Q (m^3/s) / Area (1000 km^2).

Only monitoring stations with sufficient amount of measurements are included, and here we define sufficient monitoring as an estimated average concentration per month is not estimated based on less than 4 measurements per month over a period of 20 years.

As an example, four stations from the Limfjord has been included in this paper, see Figure 16.

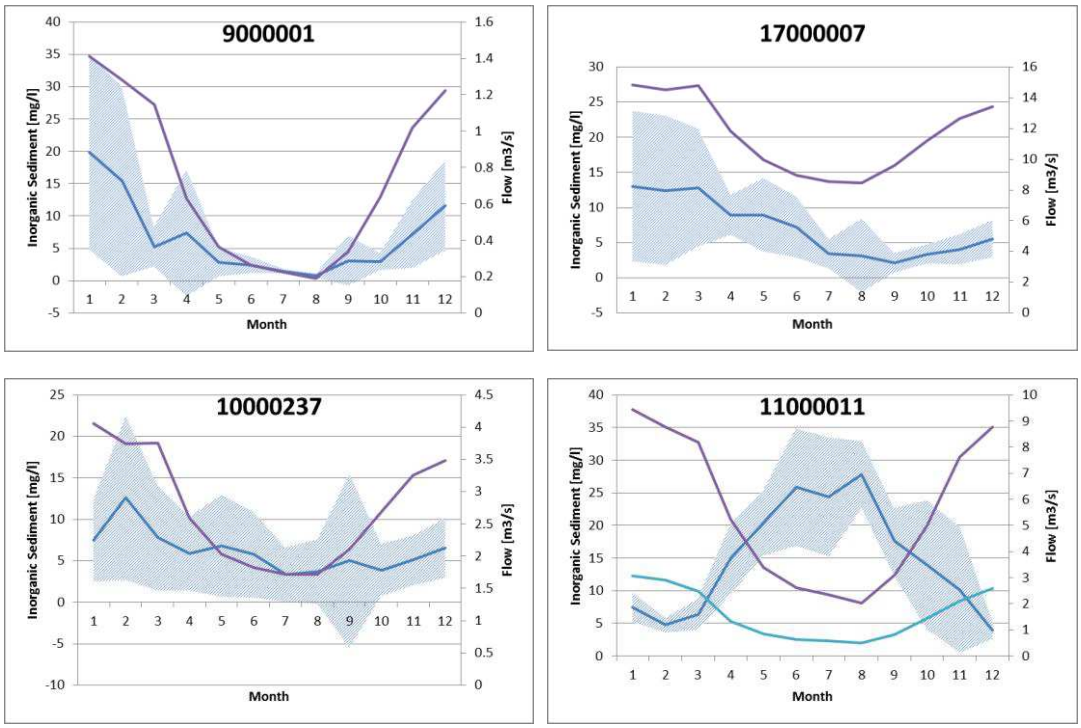


Figure 16: Monthly averages ± 1×StDev of inorganic suspended solids (SSin) at 4 different monitoring stations within the Limfjord. (Blue line) is average monthly concentrations of SSin, (blue shaded area) is ± StDev and (purple line) is average monthly discharge.

For SSin clear seasonality is observed. Especially for station 9000001 (north of Thiested bredning) the concentrations of SSin are high in fall and winter and low during summer. This is also the case for stations 17000007 (Hjarbæk fjord) and 10000238 (Halkær bredning) although not that strong as for station 9000001.

What is also clear, is the StDev being larger in autumn and winter (station 9000001 and 17000007) which indicate some relation to discharge as the discharge in these periode s can be larger, and very variable due to weather conditions (precipitation, snow and snow melt).

In Hjarbæk bredning the variance is equally large during the entire year and concentrations vary between 4-15 g/m^3.

Principles for distribution of loads

Station 11000011 (north of Nissum bredning) is included in this description as the relation to discharge is opposite to normal picture: Low discharge results in high concentrations of SSin and high discharge results in low concentrations of SSin.

For now, we have no obvious explanation for this, but the relation is adopted for streams close to this monitoring stations. In Figure 17 relations between SSin and discharge on four different monitoring stations within the Limfjord catchment is included. These kind of relations ships makes it for the F(Q/area) for the SSin estimations adopted for the mechanistic models.

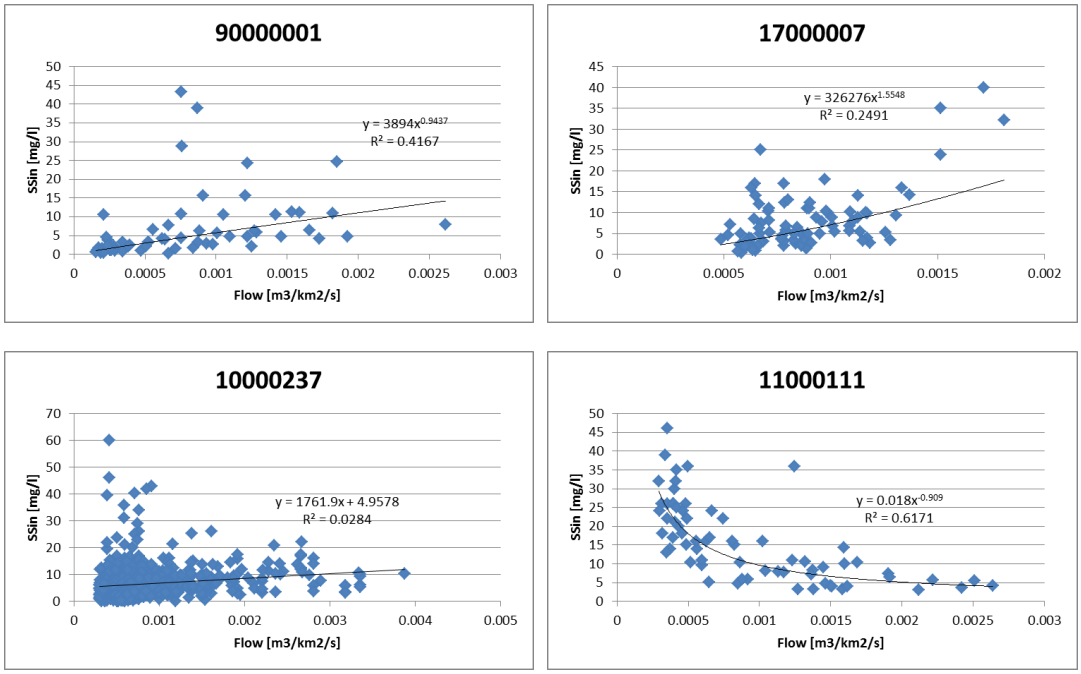
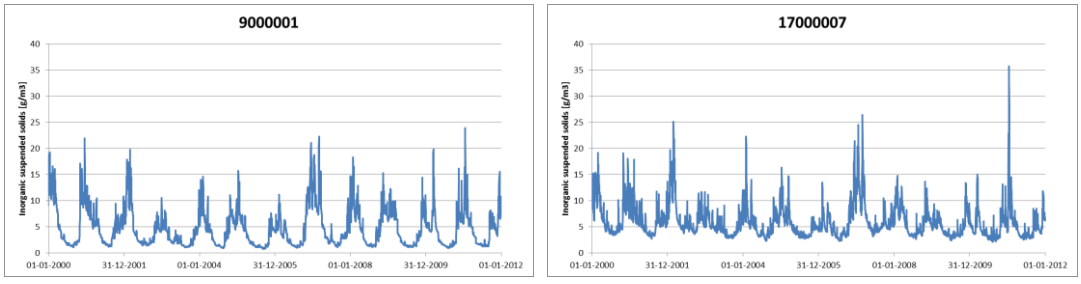


Figure 17: Relations between SSin and discharge on four different monitoring stations within the Limfjord catchment.

In Figure 17 relations between SSin and discharge (Q/area) is included. Where R^2 is larger than ~0.15 the relation is adopted for the mechanistic models whereas e.g. relation for station 10000237 does almost not exist why the average monthly concentrations is adopted instead of a relation to discharge.

Adopting the above relations results in SSin concentrations as illustrated in Figure 18. The relations build and associated statistical measures (R^2) are included in Appendix A.



Principles for distribution of loads

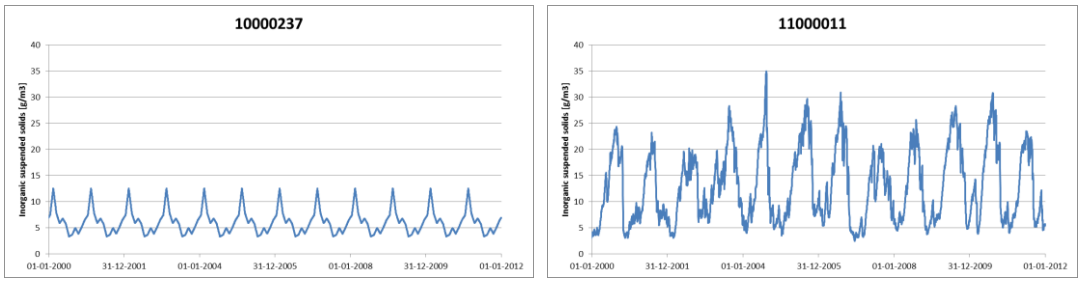


Figure 18: Examples of estimated concentrations of SSin based on relations to discharge (m^3/s) – upper panel: To average monthly concentrations (lower left panel) and a relation to discharge with opposite relationship (lower right panel).

8 References

/1/ Windolf et al

/2/ Q-distribution note

/3/ Vere, D. (2002): A Comparative Study between Loss on Ignition and Total Carbon analysis on Minerogenic Sediments. Studia Universitatis Babebolyai, Geologia, XLVII, 1, 2002, 171-182

/4/ Markager et al. 1992

/5/ Stedmon et al 2006

/6/ Ramûnas Stepanauskas, Niels O. G. Jørgensen, Ole R. Eigaard, Audrius, Vikas, Lars Tranvik, and Lars Leonardson (2002). Summer inputs of riverine nutrients to the Baltic Sea: bioavailability and eutrophication relevance. Ecological Monographs 72:579–597.

/7/ Windolf – beskrivelse af load til typefjorde

/8/ Hans T – Odense og ??

/9/ ??

Principles for distribution of loads

Appendix A: Monitoring stations and associated streams and 4th order water bodies.

North Sea

WQ station	Name	4th water body
90000001 – Storå	Klitmøller Å	1110
11000011 – Kastet Å	Thyborøn	1200
90000001 – Storå	Dybe Å	1210
90000001 – Storå	Bækmarksbro Å	1241
90000001 – Storå	Damhus Å	1242
22000062 – Storå	Storå	1243
25000086 – Tim Å	Thorsminde	1250
25000086 – Tim Å	Von Å	1310
25000086 – Tim Å	Venner Å	1321
25000086 – Tim Å	Velling Stauning Landkanal	1322
25000097 – Skjern Å	Skjern Å	1323
25000078 – Omme Å	Hvide Sande	1330
31000032 – Frisvad Møllebæk	Henne Mølleå	1410
31000027 – Varde Å	Kallesmærsk	1510
35000011 – Sneum Å	Fanø	1520
39000001 – Brøns Å	Rømø	1530
31000027 – Varde Å	Varde Å	1610
38000024 – Ribe Å	Ribe Å	1620
36000009 – Kongeåen	Kongeåen	1620
35000011 – Sneum Å	Sneum Å	1620
39000001 – Brøns Å	Brøns Å	1651 (Catchment 1630)

Principles for distribution of loads

WQ station	Name	4th water body
42000021 – Vidå	Vide Å	1651
40000001 – Brede Å	Brede Å	1651
30000002 – Uggerby Å	Skagen	2100
30000002 – Uggerby Å	Uggerby Å	2110
90000001 – Storå	Lild Strand	2200
60000001 – Ry Å	Nybæk	2213
40000005 – Liver Å	Liver Å	2213
90000021 – Tranum Å	Slette Å	2216
90000001 – Storå	Esdal Vandløb	2310

Kattegat

WQ station	Name	4th water body
5000003 – Voer Å	Lundbæk	3011
5000003 – Voer Å	Filstrøm	3012
5000003 – Voer Å	Læsø Nord	3013
23000087 – Hevring Å	Anholt	3020
48000007 – Højbro Å	Hesselø	3102
48000007 – Højbro Å	Højbro Å	3110
51000020 – Lammefjordens Pumpekanaler	Klintsø-Landkanal	3310
24000061 – Feldbæk	Hoed Å	3410
24000061 – Feldbæk	Koldingsand Nordkanal	3420
23000087 – Hevring Å	Brøndstrup Mølleå	3510
23000087 – Hevring Å	Hevring Å	3520
23000087 – Hevring Å	Lindbjerg Bæk	3531
21000467 – Gudenå	Gudenå	3532

Principles for distribution of loads

WQ station	Name	4th water body
21000413 – Alling Å	Allinge Å	3533
15000002 – Kastbjerg Å	Store Vejle Pumpekanal	3540
15000002 – Kastbjerg Å	Kastbjerg Å	3611
15000035 – Villestrup Å	Villestrup Å	3612
15000042 – Onsild Å	Onsild Å	3613
	-	3623
15000032 – Haslevgårds Å	Haslevgårds Å	3626
80000001 – Gerå	Hals	3812
80000001 – Gerå	Gerå	3814
50000003 – Voer Å	Voer Å	3816
20000005 – Elling Å	Søby Å	3910
20000005 – Elling Å	Elling Å	3920

Nordlige Bælthav

WQ station	Name	4th water body
27000035 – Odder Å	Sørende	4011
27000035 – Odder Å	Stavns Fjord	4012
27000035 – Odder Å	Samsø Nordvest	4021
27000035 – Odder Å	Sælvig	4022
27000035 – Odder Å	Dallebæk	4023
27000035 – Odder Å	Vester kanal	4023
27000035 – Odder Å	Tunø	4025
51000020 – Lammefjordens pumpekanaler	Fuglebæks Å	4110
51000020 – Lammefjordens pumpekanaler	Bølerenden	4115
51000020 – Lammefjordens	Revesgrøften	4115

Principles for distribution of loads

WQ station	Name	4th water body
pumpekanaler		
51000020 – Lammefjordens pumpekanaler	Bregninge Å	4120
51000020 – Lammefjordens pumpekanaler	Tangmoserenden	4120
51000020 – Lammefjordens pumpekanaler	Vestre Landkanal	4120
45000058 – Geels Å	Nordskov	4210
45000058 – Geels Å	Fyns Hoved	4221
45000058 – Geels Å	Sørenden	4222
45000058 – Geels Å	Hindsholm	4223
45000058 – Geels Å	Ålekisterenden	4224
45000058 – Geels Å	Gabet	4225
	Odense Fjord	4231
	Odense Fjord	4232
43000003 – Ringe Å	Storskov	4250
43000003 – Ringe Å	Ringe Å	4260
43000003 – Ringe Å	Afløb fra Tørresø	4260
43000003 – Ringe Å	Lungrenden	4270
43000003 – Ringe Å	Jesore Byrende	4270
29000009 – Rohden Å	As-Rårup Skelbæk	4310
28000001 – Bygholm Å	Skjold Å	4320
28000001 – Bygholm Å	Hjarnø	4331
27000045 – Hansted Å	Vl. S. f. Lerdrup	4332
28000001 – Bygholm Å	Glud Bæk	4332
27000045 – Hansted Å	Åkær Å	4333
27000045 – Hansted Å	Møllebæk	4333
27000045 – Hansted Å	Haldrup Mølleå	4333

Principles for distribution of loads

WQ station	Name	4th water body
28000001 – Bygholm Å	Skelbækken	4333
27000045 – Hansted Å	Hansted Å	4334
28000001 – Bygholm Å	Klokkedal Å	4334
27000035 – Odder Å	Malskær Å	4340
27000035 – Odder Å	Odder Å	4360
24000061 - Feldbæk	Egå	4411
24000061 - Feldbæk	Skæring Bæk	4411
24000061 - Feldbæk	Skødstrup Bæk	4111
24000061 - Feldbæk	Balskov Bæk	4412
24000061 - Feldbæk	Knubbro Baek	4412
24000061 - Feldbæk	Kolå	4412
24000061 - Feldbæk	Stenbæk	4420
24000061 - Feldbæk	Sletterhage	4440
26000080 – Århus Å	Giberå	4450
24000061 - Feldbæk	Vadbro Bæk	4450
26000080 – Århus Å	Århus Å	4460
24000061 - Feldbæk	Femmøller Mølleå – Skovmølle Bro - udløb	4510

Lillebælt

WQ station	Name	4th water body
43000003 – Ringe Å	Kragelund Møllebæk	5110
43000003 – Ringe Å	Ålebækken	5110
43000003 – Ringe Å	Fogense Eng	5110
43000001 – Stor Å	Stor Å	5120
43000001 – Stor Å	Aulby Mølleå	5120
29000009 – Rohden Å	5131_nn	5131
29000009 – Rohden Å	Rosenvold Å	5132

Principles for distribution of loads

WQ station	Name	4th water body
33000004 – Spang Å	Spangs Å	5132
33000004 – Spang Å	Hede Å	5133
29000009 – Rohden Å	Rohden Å	5133
29000009 – Rohden Å	Tirsbæk	5134
33000004 – Spang Å	Sellerupskov Bæk	5134
32000001 – Vejle Å	Vejle Å	5135
43000007 – Viby Å	Afløb fra Staurby Skov	5200
33000004 – Spang Å	Erritsø Bæk	5200
43000007 – Viby Å	Føns Vang	5240
37000011 – Binderup Mølleå	Tilløb Kolding Fjord_5261	5261
37000011 – Binderup Mølleå	Tilløb Kolding Fjord_5262	5262
34000019 – Kolding Å	Dalby Møllebæk	5263
34000019 – Kolding Å	Kolding Å	5263
33000004 – Spang Å	Gudsø Mølleå	5264
43000007 – Viby Å	Fønsskov	5310
43000007 – Viby Å	Laven Bæk	5320
46000001 – Brende Å	Afløb fra Grevindeskov	5330
46000001 – Brende Å	Moserenden	5330
37000036 – Kærmølle Å	Hejlsminde Strand	5340
37000038 – Vejle Å	Aller Å	5341
37000011 – Binderup Mølleå	Binderup Mølleå	5350
37000038 – Vejle Å	Brandsø	5401
46000020 – Puge Mølle Å	Bågø	5402
37000039 – Fjeldstrup Å	Årø	5403
46000020 – Puge Mølle Å	Kærum Å	5410
46000001 – Brende Å	Brende Å	5411
46000001 – Brende Å	Ålebækken	5412

Principles for distribution of loads

WQ station	Name	4th water body
46000020 – Puge Mølle Å	Puge Mølle Å	5413
46000020 – Puge Mølle Å	Torø	5414
37000034 – Haderslev Møllestrøm	Årøsund	5430
37000034 – Haderslev Møllestrøm	Haderslev Fjord	5440
37000039 – Fjeldstrup Å	Ørby Strand	5450
37000039 – Fjeldstrup Å	Knudbæk og Fjeldstrup Å	5460
37000038 – Vejle Å	Tilb Lillebælt_5470	5470
46000017 – Hårby Å	Damrenden	5510
41000016 – Strømmen	Havnbjerg	5520
37000034 – Haderslev Møllestrøm	Flovt Strand	5530
37000034 – Haderslev Møllestrøm	Bankel	5531
46000017 – Hårby Å	Helnæs	5610
46000017 – Hårby Å	Hattebækken	5621
46000017 – Hårby Å	Hårby Å	5621
46000017 – Hårby Å	Møllebækken	5622
47000001 – Hundstrup Å	Duereds Vaenge	5630
47000001 – Hundstrup Å	Lyø	5640
41000016 – Strømmen	Eskebæk	5650
41000016 – Strømmen	Melved Bæk	5660
41000016 – Strømmen	Humbæk	5660
41000014 – Fiskbæk	Kruså	5711
41000014 – Fiskbæk	Flensborg Fjord	5711
41000014 – Fiskbæk	Marbæk	5721
41000014 – Fiskbæk	Nybøl Nor	5722
41000014 – Fiskbæk	Broager Vig	5723
41000014 – Fiskbæk	Krambæk	5730

Principles for distribution of loads

WQ station	Name	4th water body
41000014 – Fiskbæk	Vemmingbugt	5731
41000016 – Strømmen	Vibæk	5732
41000016 – Strømmen	Kvl. 1, Broager	5740
41000012 – Elsted Bæk	Barsø	5801
41000016 – Strømmen	Nordborg Bæk	5810
41000012 – Elsted Bæk	Bøgelunds Bæk	5820
41000012 – Elsted Bæk	Slotsmølle Å	5820
41000020 – Blå Å	Grensbæk	5820
41000012 – Elsted Bæk	Møllebæk	5830
41000012 – Elsted Bæk	Tilb Lillebælt_5840	5840
41000012 – Elsted Bæk	Elsted Bæk	5841
41000012 – Elsted Bæk	Hoptrup Å	5850
37000034 – Haderslev Møllestrøm	Tilb Lillebælt_5860	5860
37000034 – Haderslev Møllestrøm	Halk Strand	5870
41000020 – Blå Å	Blå Å	5910
41000016 – Strømmen	Holmbæk	5910
41000016 – Strømmen	Stegsvig	5911
41000016 – Strømmen	Stolbæk Bro	5913
41000016 – Strømmen	Tilb. Augustb Fj_5920	5920
41000016 – Strømmen	Sandvig	5921
41000016 – Strømmen	Tilb. Augustb Fj_5922	5922
41000016 – Strømmen	Augustenborg Fjord	5923
41000016 – Strømmen	Tilb. Augustb Fj_5924	5924
41000020 – Blå Å	Snogbæk	5930

Storebælt

WQ station	Name	4th water body

Principles for distribution of loads

WQ station	Name	4th water body
54000002 – Fladmose Å	Agersø	6100
54000002 – Fladmose Å	Omø	6100
44000021 – Vindinge Å	Sprogø	6100
55000015 – Nedre Halleby Å	Kærby Å	6110
55000015 – Nedre Halleby Å	Nedre Halleby Å	6120
55000015 – Nedre Halleby Å	Råmosegrøften	6120
56000005 – Tude Å	Tude Å	6130
56000002 – Seerdrup Å	Hulbyrenden	6140
56000001 – Bjerge Å	Kobæk Rende	6140
64000025 – Nældevads Å	Femø	6201
64000025 – Nældevads Å	Askø	6202
62000012 – Halsted Å	Fejø	6203
54000002 – Fladmose Å	Stigsnæs	6210
56000001 – Bjerge Å	Spegerborgrenden	6211
56000001 – Bjerge Å	Noret	6212
57000055 – Saltø Å	Møllerende	6220
54000002 – Fladmose Å	Tjærebyrenden	6221
54000002 – Fladmose Å	Fladmose Å	6221
54000002 – Fladmose Å	Tørremølle rende	6222
57000055 – Saltø Å	Saltø Å	6223
57000058 – Nedre Suså	Nedre Suså	6223
57000052 – Fladså	Fladså	6223
57000052 – Fladså	Kyllebæk	6224
57000052 – Fladså	Basnæs Grøften	6224
60000032 – Næs Å	Næs Å	6225
60000029 – Køng Å	Køng Å	6225
61000011 – Sørup Å	Langkærrende	6230

Principles for distribution of loads

WQ station	Name	4th water body
61000011 – Sørup Å	T.T.Smålandshavet_6232	6232
61000011 – Sørup Å	T.T.Guldborgsund_6251_a	6251
36000007 – Saksløbing Å	T.T.Guldborgsund_6251_b	6251
36000007 – Saksløbing Å	Ny Krog Vandløb	6252
61000011 – Sørup Å	Sørup Å	6252
61000012 – Tingsted Å	Tingsted Å	6252
61000012 – Tingsted Å	Marbæk Kanal	6253
61000015 - Nordkanalen	Flintinge Å	6253
61000015 - Nordkanalen	Rørmose Bæk	6253
63000007 – Sakskøbing Å	T.T.Smålandshavet_6261	6261
63000007 – Sakskøbing Å	Låge Å	6261
63000007 – Sakskøbing Å	Sakskøbing Å	6262
63000007 – Sakskøbing Å	T.T.Smålandshavet_6262	6262
63000007 – Sakskøbing Å	Lomose Å	6262
64000025 – Nældevads Å	Nældemose Å	6262
62000012 – Halsted Å	Kasbæk	6263
62000012 – Halsted Å	Ørby Å	6263
64000025 – Nældevads Å	Stokkemarkeløbet	6263
62000015 – Marrebæksrende	Uterslevløbet	6264
60000031 – Mern Å	Vintersebølle Bæk	6311
60000031 – Mern Å	Bakkesbølle Bæk	6311
61000011 – Sørup Å	Orenæs	6312
60000031 – Mern Å	T.T.storstrømmen_6313	6313
60000034 – Sømose Bæk	Askeby Landkanal	6322
60000034 – Sømose Bæk	Bækrenden	6323
60000034 – Sømose Bæk	Damme Vandløb	6323
61000013 – Fribrødre Å	Gundslev Å	6330
61000013 – Fribrødre Å	Fribrødre Å	6330

Principles for distribution of loads

WQ station	Name	4th water body
61000013 – Fribrødre Å	Søborgkanalen	6330
62000015 – Marrebæksrende	Marrebæksrende	6420
62000017 – Ryde Å	Vestkanalen	6420
62000017 – Ryde Å	Hovedkanalen	6421
62000012 – Halsted Å	Branderslev Å	6421
62000017 – Ryde Å	Søndernor	6422
47000036 – Vejstrup Å	Akkemoserenden	6430
47000033 – Lillebæk	Troldebjerggrøften	6440
47000035 – Syltemae Å	Skelbækken	6510
47000035 – Syltemae Å	Syltemae Å	6510
47000035 – Syltemae Å	Lehnskov Bæk	6510
47000001 – Hundstrup Å	Rislebæk	6511
47000001 – Hundstrup Å	Bjerne Bæk	6511
47000001 – Hundstrup Å	Hundstrup Å	6512
47000001 – Hundstrup Å	Møllebækken	6512
47000036 – Vejstrup Å	Kobberbækken	6520
47000036 – Vejstrup Å	Halling Skov	6521
47000036 – Vejstrup Å	Egemadsafløbet	6521
47000036 – Vejstrup Å	Thurø	6522
47000036 – Vejstrup Å	Lindelse Nor	6531
47000036 – Vejstrup Å	Langeland	6532
47000035 – Syltemae Å	Tåsinge	6533
47000035 – Syltemae Å	Kløven	6541
47000035 – Syltemae Å	Landgrøften	6542
47000036 – Vejstrup Å	Skattebøllerenden	6610
47000035 – Syltemae Å	Vemmenæs	6620
47000035 – Syltemae Å	Nørreskov Bæk	6630
47000037 –	Kongshøj Å	6650

Principles for distribution of loads

WQ station	Name	4th water body
Stokkebækken		
47000037 – Stokkebækken	Stokkebækken	6650
47000036 – Vejstrup Å	Vejstrup Å	6650
47000033 – Lillebæk	Tange Å	6650
47000037 – Stokkebækken	Tåsinge Strand	6710
44000021 – Vindinge Å	Ladegårds Å	6721
44000021 – Vindinge Å	Ørbæk Å	6722
44000021 – Vindinge Å	Grønholt afløbet	6740
44000021 – Vindinge Å	Lysemoseafløbet	6740
44000021 – Vindinge Å	Kauslunde Å	6751
45000058 – Geels Å	Tårup Inddæmmede Strand	6751
45000058 – Geels Å	Vejlebækken	6752
45000058 – Geels Å	Skjoldmoserenden	6753
45000058 – Geels Å	Ålebækken	6753
45000058 – Geels Å	Hindsholm	6760

Øresund

WQ station	Name	4th water body
59000010 – Stevns Å	Møllerende	7110
59000008 – Vedskølle Å	Vedskølle Å	7122
59000006 – Tryggevælde Å	Tryggevælde Å	7122
58000047 – Køge Å	Køge Å	7124
53000010 – Lille Vejle Å	Lille Vejle Å	7126
53000054 – Skensved Å	Skensved Å	7126
53000054 – Skensved Å	Solrød Bæk	7126
53000054 – Skensved Å	Karlstrup Mosebæk	7126

Principles for distribution of loads

WQ station	Name	4th water body
53000010 – Lille Vejle Å	Olsbæk	7126
53000011 – Store Vejle Å	Store Vejle Å	7127
53000028 – Harrestrup Å	Harrestrup Å	7128
53000028 – Harrestrup Å	Hovedgrøften	7128
53000028 – Harrestrup Å	Enghave Å	7130
53000028 – Harrestrup Å	Saltholm	7201
53000028 – Harrestrup Å	Kastrup	7210
50000051 – Mølle Å	Tårbæk Rende	7220
50000051 – Mølle Å	Mølle Å	7220
50000048 – Kighanerenden	Kighanerenden	7220
50000057 – Nive Å	Nive Å	7230
50000048 – Kighanerenden	Ulvemoserenden	7230
50000057 – Nive Å	Humlebækken	7230
50000057 – Nive Å	Krogerup vandløb	7230
50000057 – Nive Å	Egebæk	7230
50000056 – Nive Å	Helsingør Red	7240
48000011 – Østerbæk	Knudemoseløbet	7310
48000004 – Esrum Å	Esrum Å	7320
48000004 – Esrum Å	Pandehave Å	7320
48000011 – Østerbæk	Vesterbæk	7320
48000011 – Østerbæk	Østerbæk	7320
48000010 – Søborg Kanal	Søborg Kanal	7330

Sydlige Bælthav

WQ station	Name	4th water body
47000035 – Syltemae Å	Magleby Nors Pumpekanal	8110

Principles for distribution of loads

WQ station	Name	4th water body
65000001 – Rødby Fjord	Rødby Fjord	8210
61000015 – Nordkanalen	Ålholmløbet	8220
61000015 – Nordkanalen	Egeholmløbet	8220
61000015 – Nordkanalen	T.T.Lambo Farvand_8220_a	8220
61000015 – Nordkanalen	Strognæs Bæk	8220
61000015 – Nordkanalen	Pumpekanal Strognæs Enge	8220
61000015 – Nordkanalen	T.T.Lambo Farvand_8220_b	8220
61000015 – Nordkanalen	T.T.Lambo Farvand_8220_c	8220

Østersø

WQ station	Name	4th water body
66000014 – Bagge Å	Vase Å	9100
66000014 – Bagge Å	Byå	9110
66000014 – Bagge Å	Blykobbe Å	9120
66000014 – Bagge Å	Kobbe Å	9130
66000014 – Bagge Å	Øle Å	9140
66000014 – Bagge Å	Læså	9150
61000012 – Tingsted Å	Askehaveløbet	9210
60000034 – Sømosebæk	Nyhåndsbæk	9220
60000036 – Tubæk	Brønsvig	9300
60000034 – Sømosebæk	Sømosebæk	9310
60000034 – Sømosebæk	Ulvshale Bækken	9320
60000034 – Sømosebæk	Landsledgrøft	9321
60000031 – Mern Å	Mern Å	9330
60000026 – Herredsbæk	Herredsbæk	9350
60000036 – Tubæk	Tubæk	9350
60000024 – Fakse Å	Fakse Å	9360

Principles for distribution of loads

WQ station	Name	4th water body
60000037 – Vivede Mølleå	Vivede Mølleå	9360

Limfjord:

Estimating the fraction of dissolved inorganic nutrients to total nutrient is based on monitoring data from following water quality stations. Also, the streams covered by each station and corresponding 4th order water body in included.

WQ station	Name	4th water body
17000007 - Simested	Simested Å	3745
18000077 - Skals Å	Skals Å	3745
19000011 - Fiskbæk Å	Fiskbæk Å	3745
19000012 - Jordbro Å	Jordbro Å	3745
13000005 - Lerckenfeld Å	Lerkenfeld Å	3743
13000010 - Trend Å	Trend Å	3741
	Stistrup Å	3742
16000030 - Lyby-Gronning Grøft	Astrup Bæk	3742
20000024 - Karup Å	Karup Å	3747
12000001 - Vejerslev Bæk	Mygdam Å	3764
	Spang Å	3763
	Lyngbro Bæk	3763
16000023 - Bredkær Bæk	Skærbæk Å	3754
	Hellegård Å	3754
	Hummelmose Å	3754
16000024 - Fold Å	Fold Å	3771
	Østergård Bæk	3772
16000070 - Vium Mølleå	Vium Mølleå	3751
	Hinnerup Å	3734
	Rødding Å	3752

Principles for distribution of loads

WQ station	Name	4th water body
9000001 - Storå	Sundby Å	3762
	Storå	3761
	Sløjkanal	3733
	Ørebro Kanal	3732
10000013 - Dybvad Å	Dybvad Å	3731
	Vaar Å	3728
11000011 - Hvidbjerg Å	Kastet Å	3773
	Serup Å	3753
	Borregår Bæk	3753
13000065 - Bjørnsholm Å	Bjørnsholm Å	3733
7000002 - Lindholm Å	Ry å	3722
	Lindenholm Å	3721
	Lerbæk	3719
	Stae Bæk	3717
9000021 - Tranum Å	Tranum Å	3726
10000009 - Herreds Å	Halkær Å	3724
10000014 - Binderup Å	Binderup Å	3723
10000010 - Kærs Mølleå	Kærs Mølleå	3721
10000011 - Romdrup Å	Romdrup Å	3715
14000016 - Lindenborg Å	Lindenborg Å	3713
	Hyllebrors Bæk	3711

Estimating the concentration of inorganic suspended sediments (SSin) is based on monitoring data from following water quality stations. Also, the streams covered by each station and corresponding 4th order water body in included.

WQ station	Name	4th water body	SSin estimations
17000007 - Simested	Simested Å	3745	$y = 326276x^{1.5548}$ ($R^2 = 0.2491$)

Principles for distribution of loads

WQ station	Name	4th water body	SSin estimations
	Lerkenfeld Å	3743	
18000077 - Skals Å	Skals Å	3745	Monthly mean
19000012 - Jordbro Å	Jordbro Å	3745	$y = 166938x^{1.453}$ ($R^2 = 0.1621$)
	Fiskbæk Å	3745	
20000024 - Karup Å	Karup Å	3747	y = 20795x1.1814 ($R^2 = 0.1568$)
16000030 - Lyby-Gronning Grøft	Astrup Bæk	3742	$y = 3E+08x^{2.5228}$ ($R^2 = 0.3743$)
13000010 - Trend Å	Trend Å	3741	$y = 5124.8x^{1.0339}$ ($R^2 = 0.1452$)
	Stistrup Å	3742	
	Bjørnsholm Å	3733	
16000070 - Vium Mølleå	Vium Mølleå	3751	$y = 1.8945e^{683.09x}$ ($R^2 = 0.3582$)
	Hinnerup Å	3734	
	Rødding Å	3752	
	Mygdam Å	3764	
	Spang Å	3763	
	Lyngbro Bæk	3763	
16000024 - Fold Å	Fold Å	3771	$y = 20795x^{1.1814}$ ($R^2 = 0.1568$)
	Østergård Bæk	3772	
	Skærbæk Å	3754	
	Hellegård Å	3754	
	Hummelmose Å	3754	
11000011 - Hvidbjerg Å	Kastet Å	3773	$y = 0.018x^{-0.909}$

Principles for distribution of loads

WQ station	Name	4th water body	SSin estimations
			(R^2 = 0.6171)
	Serup Å	3753	
	Borregår Bæk	3753	
9000001 - Storå	Sundby Å	3762	$y = 3894x^{0.9437}$ (R^2 = 0.4167)
	Storå	3761	
	Sløjkanal	3733	
	Ørebro Kanal	3732	
9000021 - Tranum Å	Tranum Å	3726	$y = 2.2915e^{554.03x}$ (R^2 = 0.4087)
10000237 - Halkær Å	Halkær Å	3724	Monthly mean
	Dybvad Å	3731	
	Vaar Å	3728	
	Binderup Å	3723	
7000002 - Lindholm Å	Ry å	3722	$y = 3.1223e^{505.58x}$ (R^2 = 0.179)
	Lindenholm Å	3721	
	Lerbæk	3719	
	Stae Bæk	3717	
14000016 - Lindenborg Å	Lindenborg Å	3713	Monthly mean
	Romdrup Å	3715	
	Kærs Mølleå	3721	
	Hyllebrors Bæk	3711	

Odense Fjord:

WQ station	Name	4th water body

Principles for distribution of loads

WQ station	Name	4th water body
43000003 – Ringe Å	fj_n	4231
43000003 – Ringe Å	fj_s	4231
45000058 – Geels Å	u28	4231
45000058 – Geels Å	u29	4231
45000058 – Geels Å	u46	4231
45000058 – Geels Å	Geel	4232
	lu_n	4232
45000002 – Odense Å	oden	4232
45000002 – Odense Å	Odense_A_Discharge	4232
45000005 – Stavis	stav	4232
	u27	4232
	u48	4232
45000048 – Vejrup	vejr	4232

Roskilde/Ise Fjord

WQ station	Name	4th water body
49000054 – Arresø Kanal	Arresø	3221
49000054 – Arresø Kanal	Melby	3221
52000025 – Græse Å	Græse	3222
52000029 – Havelse	Havelse	3222
52000025 – Græse Å	Hornsherred	3222
52000033 – Mademose	Mademose	3223
52000035 - Udesundby	Sillebro	3223
52000039 – Værebro	Værebro	3223
52000063 – Hove	Hove	3224
52000199 – Maglemose	Maglemose	3224
52000199 – Maglemose	Sønderby	3224
52000068 – Langvad	Langvad	3226

Principles for distribution of loads

WQ station	Name	4th water body
52000068 – Langvad	Honepil	3227
52000068 – Langvad	Lejrerende	3227
52000068 – Langvad	Lejre Å	3227
52000068 – Langvad	Lundby	3227
52000068 – Langvad	Ørbæk	3227
52000068 – Langvad	Selsø	3227