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Variations in the elemental ratio of organic matter in the central Baltic Sea: Part II – Sensitivities of annual mass flux estimates to model parameter variations

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ABSTRACT

This study describes a sensitivity analysis that allows the parameters of a one-dimensional ecosystem model to be ranked according to their specificity in determining biochemical key fluxes. Key fluxes of interest are annual (a) total production (TP), (b) remineralization above the halocline (RM), and (c) export at 50 m (EX) at the Baltic Sea monitoring site BY15 located in the Gotland Deep basin. The model resolves mass flux of carbon (C), nitrogen (N), and phosphorous (P), while considering nitrogen fixation explicitly. Our first null hypothesis is that the variation of the value of every single model parameter affects each annual C, N, and P budget simultaneously. Our second null hypothesis states that the variation of every parameter value induces changes at least in either of the annual C, N or P budgets. Our analyses falsify both null hypotheses and reveal that 8 out of 36 parameters must be regarded redundant, as their variation neither alter annual key fluxes nor produce considerable time-shifts in model trajectories at the respective site. Seven parameters were found to induce substantial changes in annual C, N, and P flux estimates simultaneously. The assimilation efficiency of zooplankton turned out to be of vital importance. This parameter discriminates between the assimilation and destruction of algal prey during grazing. The fraction of unassimilated dead algal cells is critical for the amount of organic matter exported out of the euphotic zone. The maximum cellular N:C quota of diazotrophs and the degradation/hydrolysis rate of detrital carbon are two parameters that will likely remain unconstrained by time series data, but both affect the annual C budget considerably. Overall, our detailed specification of model sensitivities to parameter variations will facilitate the formulation of a well-posed inverse problem for the estimation of C, N and P fluxes from stock observations at the Gotland Deep.

1. Introduction

Process-oriented ecosystem modeling has become standard practice in data synthesis, state description, and future projection. In the fields of biological oceanography and aquatic ecology, ecosystem models provide solutions that can explain observations of laboratory, mesocosm, or field experiments, thereby shedding light on complex plankton interactions. In marine biogeochemistry, modeling is less subtle in terms of resolving ecological details in plankton dynamics. Of primary interest instead is the estimation of matter flux in space over an extended period (e.g. seasonal or annual carbon flux), often achieved with coupled physical–biological models. Most fluxes cannot be measured directly and are derived in consideration of certain model assumptions.

The credibility of a model to provide good biogeochemical flux estimates is often confirmed by comparison of simulation results with oceanic or limnic field data in time and space. Typical available field data are standing stock observations like concentrations of chlorophyll-*a* or of particulate organic carbon. On the one hand the simulation of model counterparts to these available observations involves uncertainties in the description of physical environmental conditions (e.g. turbulent mixing). On the other hand, uncertainties in model results also depend on the parameter values chosen for simulation, which is an ever side aspect of ecosystem- and biogeochemical modeling. Model parameter values can be constrained by fitting the results of an ecosystem model to standing stock data in time and space (e.g. Fasham and Evans,

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1995). Accordingly, good model fits to observations are expected to also yield reliable flux estimates. But this expectation is often diminished, given the fact that there is a lack of verified data on the precise mechanisms of plankton dynamics or on the feasibility of aggregating diverse plankton species into single groups. Anderson (2005) highlights the necessity and value of uncertainty analyses in marine ecosystem modeling, in particular if phytoplankton functional groups are introduced. Notwithstanding this, sensitivity and uncertainty analyses of aquatic and marine ecosystem models have been insufficiently addressed in the past (e.g. Arhonditsis and Brett, 2004).

For a perfect model, the question is whether available data suffice to constrain all the model's parameter values, which would then provide a unique solution of matter flux, e.g. of total annual net primary production. But ecosystem models are far from being perfect and therefore information about the model itself (like its complexity) is required as *a priori* input to elaborate any data assimilative approach to parameter optimization. Hemmings and Challenor (2012) suggested to differentiate between uncertainties that derive from environmental forcing applied in the model and uncertainties that are solely associated with model structure, i.e. number and type of parameterizations. These intrinsic structural uncertainties can be artificially created simply by introducing more parameterizations to a model.

To date, a vast number of experiments have exhibited detailed changes in the physiology and composition of plankton in response to environmental variations. For modelers it is tempting to increase model complexity to account for these responses. Nevertheless, it can be misleading to expand the model's complexity so that the number of biological interactions (parameterizations) is increased, since this usually aggravates the problem of uncertainty in model solution, including aspects of stability and periodicity (Denman, 2003). Although variability in space and time may appear better resolved after the addition of a new process, the question remains whether the addition improves flux estimates as well. Evans (1999) points out that model refinements and data assimilation should be approached iteratively in order to improve flux estimates. In the situation where a specific process is considered relevant, ecosystem modelers can easily be caught between adding a qualitative description of this process and the necessity of finding sufficient quantitative constraints for a unique model solution. It is difficult to communicate this discrepancy between modelers and observers, but clarification can be achieved if there is the motivation in model-sensitivity analyses to demonstrate the benefits and limitations of ecosystem- and biogeochemical modeling.

Our study describes a procedure for model-sensitivity analysis that does not necessarily require observational data but is conditioned by the model's structure and parameterizations. In this way, the analysis exhibits valuable information about the model itself. Analyses of this type reveal the degree of model redundancy. They may also help to identify the data needed to constrain model flux estimates. Uncovering model redundancy may justify the downgrading of complexity without loss of credibility in flux estimation. Such justification is critical, because the mathematical rationale of excluding parameterizations from a model sometimes contradicts the opinions and hypotheses of ecologists and biogeochemists.

Our major objective is to identify predominant, as well as redundant, control parameters of the model applied in Kreus et al. (accompanying paper, same issue). The model was primarily devised to determine differences between mass flux estimates of carbon (C), nitrogen (N) and phosphorus (P), while explaining time series data of nutrients, particulate matter, and carbon dioxide partial pressure. With our analysis presented here we want to specify model parameters according to their effects on annual fluxes (key fluxes) at the Baltic Sea, HELCOM monitoring site BY15

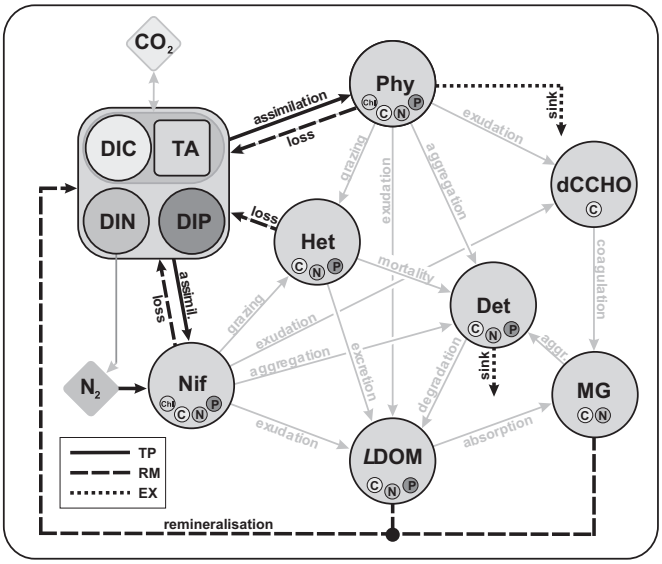

Fig. 1. Sketch of model compartments together with arrows that depict fluxes between them. Those fluxes that are considered for the calculation of key fluxes are marked separately: total production (TP) solid black lines; remineralization (RM) dashed black lines; and vertical export (EX) dotted black lines.

Gotland Deep. The key fluxes of interest are total production, remineralization within the upper euphotic zone, and export at 50 m, which is the approximate depth of the permanent halocline at BY15. High oxygen levels are maintained down to 50 m and ecosystem processes that induce noticeable denitrification can be neglected. Key fluxes are distinguished further between elements C, N and P respectively, as depicted in Fig. 1. We state the null hypothesis that all model parameters affect annual C, N and P budgets simultaneously. We anticipate, however, that many model parameters have irregular effects on C, N and P cycling, whereas few are expected to constrain either of the C, N or P budgets individually.

Overall, our analysis can be interpreted as an expedient preceding step before applying a more elaborate parameter optimization method, as we provide prior information about model sensitivities to parameter variations. This study offers a general discussion on the discrimination between chemical species, on model complexity, and on the sensitivities of flux estimates when changing parameter values.

2. Method

For the analysis we resume the one-dimensional model setup described in Kreus et al. (accompanying paper, same issue). Briefly, Kreus et al.'s one-dimensional ecosystem model was devised for a local site in the Baltic Sea, specifically for the Helsinki Commission (HELCOM) monitoring site BY15 in the Baltic Proper. The location for the model was chosen because of an existing physical model setup. This setup is based on a one-dimensional (1D) simulation with the general ocean turbulence model (GOTM) that was tested and confirmed for the Baltic Sea monitoring site BY15 by Burchard et al. (2006). To account for effects due to horizontal advection in their GOTM setup, the physical state variables like salinity and temperature were also nudged to observed vertical profiles, which assured mixing depths close to reality. The original number of vertical layers in the setup of Burchard et al. (2006) was decreased from 30 to 15 within the upper 50 m of the water column, mainly to reduce computational time of the coupled biogeochemical model that resolves 24 biological and chemical state variables. With the coupled physical–biological model setup we focus on