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Testing a marine ecosystem model: sensitivity analysis and parameter optimization

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Abstract

A data assimilation technique is used with a simple but widely used marine ecosystem model to optimize poorly known model parameters. A thorough analysis of the a posteriori errors to be expected for the estimated parameters was carried out. The errors have been estimated by calculating the Hessian matrices for different problem formulations based on identical twin experiments. The error analysis revealed inadequacies in the formulation of the optimization problem and insufficiencies of the applied data set. Modifications of the actual problem formulation, which improved the accuracy of the estimated parameters considerably, are discussed.

The optimization procedure was applied to real measurements of nitrate and chlorophyll at the Atlantic Bermuda site. The parameter optimization gave poor results. We suggest this to be due to features of the ecosystem that are unresolved by the present model formulation. Our results emphasize the necessity of an error analysis to accompany any parameter optimization study. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Marine ecosystem; Sensitivity analysis; Parameter optimization

1. Introduction

Within the scope of global climate studies, the modeling community is seeking marine ecosystem models capable of describing wide regions of the oceans. Models should be robust and behave equally well in different biogeochemical provinces of the global ocean. These range from temperate and high latitude systems, which may be viewed as a linear food chain, to oligotrophic systems, characterized by high overturning rates and a food net dominated by the microbial loop. Parameterizations appropriate to represent these different types of ecosystems are needed for basin-wide and global ocean models. The parameters in marine ecosystem models are generally poorly known quantities. This is mainly due to the fact that the model state variables are highly integrated pools that comprise different species, which are affected differently by biotic and abiotic changes in their environment. The model parameters should represent the integrated behavior of this heterogenic mixture of species. Furthermore, the proportions of the different species contributing to the species pool may change in time as ecosystems respond to changes in environmental conditions.

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Thus, the model parameters are not straightforward to define.

The parameter values are difficult to determine by measurements. Single quantities like phytoplankton growth rates may be found by laboratory experiments. However, these values represent mostly single species under controlled conditions and their application to the in situ conditions is questionable. Only until recently, the general procedure for setting parameters of ecological models was to use corresponding values from former modeling studies and/or fit the model output to observed data by subjective tuning of the parameters. The employment of data assimilation techniques seems an attractive alternative, since these methods allow one to settle poorly known model parameters objectively based on statistical assumptions about observations of the real system. Such a parameter estimation is done by combining the dynamical model and measurements of the state of the real system. The data assimilation technique generally used within the context of parameter optimization is the adjoint method (Lawson et al., 1995, 1996; Schartau et al., 2000; Spitz et al., 1998, 2000). A few studies employ simulated annealing (Hurtt and Armstrong, 1996, 1999; Matear, 1995) or a non-linear optimization technique (Evans, 1999; Fasham and Evans, 1995; Prunet et al., 1996a,b) to perform parameter optimizations. The basic idea underlying these methods is to vary model parameters until the misfit between the dynamical model and the time-distributed data is minimized, while the model equations are fulfilled exactly. The general procedure of parameter estimation by the adjoint method is discussed in detail by Evensen et al. (1998).

Former assimilation studies demonstrate that the optimization of ecological parameters is a difficult task. While the feasibility of the adjoint method to recover model parameters was shown in principle by identical twin experiments (Lawson et al., 1996; Schartau et al., 2000; Spitz et al., 1998), the application to real observations turned out to be problematic. For instance, Fasham and Evans (1995) did not find a parameter set that would give a good fit to the whole observation set simultaneously, Prunet et al. (1996a) found only a few model parameters to be constrained by the data, and Spitz et al. (1998) could not estimate the optimal model parameters when employing real observations.

Since an optimization procedure can only provide estimates of the parameters in question, we regard studies of this kind as not complete without an analysis of the errors of the optimal estimate. This paper provides a thorough investigation of the errors to be expected for the optimal parameter estimates. The important problem of what aspects of the parameter set are difficult to determine or are not constrained by the available data is illuminated by an error analysis. The estimated a posteriori errors inspire modifications of the problem formulation and reveal the inadequacies in the employed data sets and model formulation. Since the error analysis is based on a widely used modeling approach, the results apply to a whole class of presently used ecological models.

The ecological model, the inverse formulation, and the method to obtain the error estimates are described in Section 2. The error analysis is presented and discussed in Sections 3 and 4, respectively. An application of the optimization procedure to real observations is performed in Section 5, followed by its discussion in Section 6. The paper concludes with Section 7.

2. Method

2.1. The ecological model

The ecosystem model employed in this study is a simple representation of the nitrogen cycle, but nevertheless a widely used approach to describe the pelagic system of marine environments. The model consists of four partial differential equations that determine the dynamical evolution of the state variables: dissolved inorganic nutrients DIN, phytoplankton Phy, zooplankton Zoo and detritus Det. This type of model is also termed the NPZD-model. A schematic of the model is given in Fig. 1. NPZD-models are currently used in various spatial resolutions ranging from vertically integrated and one-dimensional models (Doney et al., 1996; Evans and Parslow, 1985; Fennel, 1995) to coupled three-dimensional models (Fennel, 1999; Oschlies and Garçon, 1998, 1999; Palmer and Totterdell, 1999). While the conceptual structure of the ecological part of all of these models is very similar, slight differ-

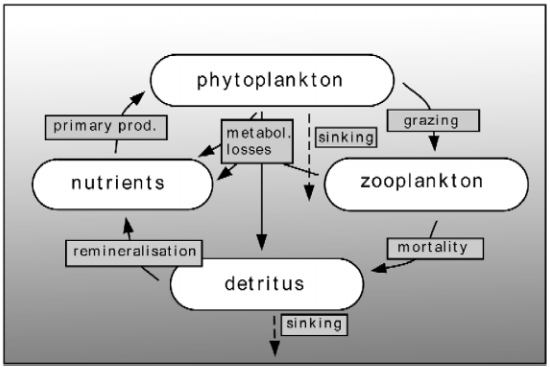


Fig. 1. Schematic of the NPZD-model.

ences occur in the explicit mathematical formulation of the process parameterizations. The latter are empirical and thus depend to some extent on the personal choice of the modeler.

This study is based on a vertically integrated formulation of the model, that is, the state variables are assumed to be homogenously distributed over the mixed layer. The evolution of the mixed layer is calculated from prescribed daily mixed layer depths (MLD). The prescribed mixed layer depths are taken from a simulation of the general circulation model described by Drange (1996). The circulation model is a version of the Miami Isopycnic Coordinate Ocean Model (MICOM) (Bleck et al., 1992) employing the mixed layer parameterization of Gaspar (1988) and forced with ECMWF wind stresses, heat fluxes and solar radiation. The positive change of the mixed layer depth $h^{+}(t)$ determines the rate of nutrient entrainment into the mixed layer from greater depths. It is given by

$$h^{+}(t) = \max(h(t),0),$$

$$\text{where} \quad h(t) = \frac{\mathrm{dMLD}}{\mathrm{d}t}. \tag{1}$$

The phytoplankton growth rate g_{P} depends on the supply of dissolved inorganic nutrients DIN according to a linear Michaelis–Menten kinetic and on the availability of photosynthetically active light $F(I)$. The growth rate is given by

$$g_{\mathrm{P}}(I,\mathrm{DIN}) = \mu_{\mathrm{P}} \frac{\mathrm{DIN}}{k_{\mathrm{N}} + \mathrm{DIN}} \cdot \frac{1}{\mathrm{MLD}} \int_{0}^{\mathrm{MLD}} F(I)\,\mathrm{d}z, \tag{2}$$

where μ_{P} is the maximum phytoplankton growth rate, k_{N} the half-saturation concentration for nutrient uptake and I the depth dependent radiation. The photosynthesis to light relationship (PI-curve) is determined following Evans and Parslow (1985)

$$F(I) = \frac{\alpha \cdot \mathrm{par} I}{\sqrt{\mu_{\mathrm{P}}^{2} + \alpha^{2} \mathrm{par}^{2} I^{2}}}. \tag{3}$$

Here α represents the initial slope of the PI-curve and par is a constant determining the fraction of incident light that is available for photosynthesis. The phytoplankton loss terms comprise grazing by zooplankton g_{Z} and linear metabolical losses due to the constant respiration and mortality rates λ_{PN} and λ_{PD}, respectively. The zooplankton grazing is represented by a squared Michaelis–Menten response

$$g_{\mathrm{Z}} = \mu_{\mathrm{Z}} \frac{\mathrm{Phy}^{2}}{k_{\mathrm{P}} + \mathrm{Phy}^{2}}, \tag{4}$$

where μ_{Z} is the maximum grazing rate and k_{P} the half-saturation concentration for phytoplankton ingestion. Zooplankton exudation is described by a constant rate λ_{ZN} while zooplankton mortality is assumed to be quadratically dependent on the zooplankton standing stock, that is $\lambda_{\mathrm{ZD}}\mathrm{Zoo}^{2}$. Detrial particles are remineralized in the mixed layer at a constant rate λ_{DN} and sink out of the mixed layer at a constant velocity w_{D}.

With these definitions, the model equations read explicitly

$$\frac{\mathrm{dPhy}}{\mathrm{d}t} = g_{\mathrm{P}}\mathrm{Phy} - g_{\mathrm{Z}}\mathrm{Zoo} - \lambda_{\mathrm{PN}}\mathrm{Phy} - \lambda_{\mathrm{PD}}\mathrm{Phy} - \frac{m + h^{+}(t)}{\mathrm{MLD}}\mathrm{Phy} \tag{5}$$

$$\frac{\mathrm{dZoo}}{\mathrm{d}t} = g_{\mathrm{Z}}\mathrm{Zoo} - \lambda_{\mathrm{ZN}}\mathrm{Zoo} - \lambda_{\mathrm{ZD}}\mathrm{Zoo}^{2} - \frac{h(t)}{\mathrm{MLD}}\mathrm{Zoo} \tag{6}$$

$$\frac{\mathrm{dDIN}}{\mathrm{d}t} = -g_{\mathrm{P}}\mathrm{Phy} + \lambda_{\mathrm{PN}}\mathrm{Phy} + \lambda_{\mathrm{ZN}}\mathrm{Zoo} + \lambda_{\mathrm{DN}}\mathrm{Det} + \frac{m + h^{+}(t)}{\mathrm{MLD}}\left(N_{\mathrm{slope}}\mathrm{MLD} - \mathrm{DIN}\right) \qquad (7)$$

$$\frac{\mathrm{dDET}}{\mathrm{d}t} = \lambda_{\mathrm{PD}}\, Phy + \lambda_{\mathrm{ZD}}\mathrm{Zoo}^{2} - \lambda_{\mathrm{DN}}\mathrm{Det} - \frac{m + h^{+}(t) + w_{\mathrm{D}}}{\mathrm{MLD}}\mathrm{Det}. \qquad (8)$$

The last terms of Eqs. (5)–(8) account for the physical processes of nutrient entrainment, dilution and mixing (Evans and Parslow, 1985). Dissolved inorganic nutrients, phytoplankton and detritus are mixed at the constant mixing rate m across the lower face of the mixed layer and are diluted if the mixed layer deepens by h^{+}. Zooplankton Zoo is assumed to maintain its position in the mixed layer and thus is diluted if the mixed layer deepens and concentrated if the mixed layer depth decreases. Nutrients are entrained from greater depths during deepening of the mixed layer. The deep nutrient concentrations are described by assuming a linear increase N_{slope} with depth (Hurtt and Armstrong, 1996). The model parameters are given in Table 1.

The model presented here is very similar to the formulations of Oschlies and Garçon (1998, 1999) and Doney et al. (1996) who also employ a linear Michaelis–Menten response for phytoplankton growth and a squared response for zooplankton grazing. The zooplankton mortality is represented by a quadratic rate in their models as well.

2.2. The inverse formulation

The idea underlying the inverse parameter optimization is to combine the simulated model dynamics with the available information about the real system, that is a set of observations. Based on the assumption that the validity of the model parameters depends on the match between the observed data and the model equivalents of these data, we search for a set of parameters that provides the best fit of the model dynamics to the observations. The search for an optimal parameter set is performed by minimizing a cost function that measures the misfit between the data and the model equivalents of the data in a least squares sense. The cost function is generally of the form

$$F(\vec{p}) = \frac{1}{2}\sum_{i}\left(\frac{X_i^{\mathrm{obs}} - X_i^{\mathrm{sim}}(\vec{p})}{\sigma_i}\right)^{2}, \qquad (9)$$

where $\vec{p}$ represents the vector of the unknown parameters. The misfit between the observations X_i^{obs} and the corresponding simulated model variables

Table 1
Initial guess of model parameters

Parameter	Symbol	Initial value	Unit
Phytoplankton maximum growth rate	μ_{P}	1.0	day^{-1}
Half-saturation value for phytoplankton growth	k_{N}	0.25	$\mathrm{mmol\ N\ m}^{-3}$
Phytoplankton mortality rate	λ_{PD}	0.05	day^{-1}
Phytoplankton respiration rate	λ_{PN}	0.05	day^{-1}
Zooplankton maximum growth rate	μ_{Z}	2.0	day^{-1}
Half-saturation value for zooplankton growth	k_{P}	0.5	$(\mathrm{mmol\ N})^{2}\ \mathrm{m}^{-6}$
Zooplankton mortality rate	λ_{ZD}	0.05	$(\mathrm{mmol\ N\ m}^{-3})^{-1}\mathrm{day}^{-1}$
Zooplankton exudation rate	λ_{ZN}	0.05	day^{-1}
Remineralisation rate	λ_{DN}	0.05	day^{-1}
Initial slope of the PI-curve	α	0.025	$(\mathrm{W\ m}^{-2})^{-1}\ \mathrm{day}^{-1}$
Photosynthetic active fraction of light	par	0.43	dimensionless
Detritus sinking rate	w_{D}	1.0	$\mathrm{m\ day}^{-1}$
Cross thermocline mixing	m	0.25	$\mathrm{m\ day}^{-1}$
Slope of nitrate concentration below the thermocline	N_{slope}	0.016	$\mathrm{mmol\ N\ m}^{-4}$

The initial parameter guess agrees with values in common use (compare Oschlies and Garçon, 1999; Doney et al., 1996; Fasham et al., 1990).

$X_i^{\mathrm{sim}}(\vec{p})$ is weighted by the inverse of the assumed a priori error σ_{i}. A minimization algorithm is applied to search for the minimum of the cost function. Every minimization step requires the computation of the gradient of the cost function with respect to the model parameters. Basically, the parameter optimization is an iteration of the following three steps.

(A) A forward model integration: the forward model (described in Section 2.1) calculates the evolution of the model state variables in time. Note that the initial conditions and the physical forcing are prescribed. Thus, the model dynamics are solely determined by the choice of the model parameters. The parameters are called independent variables or control variables in this context while the model state variables are dependent variables.

(B) An integration of the adjoint model: the adjoint model calculates the gradient of the cost function with respect to the model parameters. We used the Tangent linear and Adjoint Model Compiler (TAMC), a source-to-source translator for FORTRAN programs (Giering, 1997), as a convenient tool to obtain the adjoint model code.

(C) An optimization step: a minimization is performed in the direction of the gradient of the cost function that was computed in step B. We applied the quasi-Newton method implemented in the M1QN3 routine of the MODULOPT library (Gilbert and Lemaréchal, 1989).

This procedure is iterated until the gradient of the cost function is sufficiently small. Since the model is non-linear it is desirable to start the iteration near the global minimum in order to prevent the descent algorithm from being caught in a local minimum. Since this can be hard to judge in practice, it may become necessary to start a number of minimizations from different initial parameter sets.

2.3. The Hessian matrix

Important aspects of the problem formulation can be revealed by an investigation of the Hessian matrix of the cost function. Near the global minimum, the inverse of the Hessian matrix provides a good approximation of the covariance matrix for the independent model parameters (Thacker, 1989). The condition number of the Hessian, which is defined as the ratio of its largest to its smallest eigenvalue, determines the rate of convergence of the minimization algorithm and indicates how singular the problem is. For large condition numbers, the matrix is ill conditioned and nearly singular, whereas values close to unity characterize a well-conditioned matrix. The inverse eigenvalues of the Hessian are the errors of combinations of the estimated model parameters. These combinations are determined by the corresponding eigenvectors. The product of the eigenvectors and corresponding eigenvalues are also called parameter resolution. In the case of large inverse eigenvalues, meaning large uncertainties, some of the model parameter combinations can only poorly be determined by the data.

The Hessian of the cost function can be approximated by independently perturbing the control variables by a small amount and calculating the gradient of the cost function for each perturbation. The elements of the Hessian result in

$$h_{ij} = \frac{1}{2\Delta p_j}\left(\partial F\left(\vec{p} + \Delta p_j\right)/\partial p_i - \partial F\left(\vec{p} - \Delta p_j\right)/\partial p_i\right). \tag{10}$$

Since this finite difference method can be dependent on the choice of the Δp_j's, we have chosen to use the TAMC (Giering, 1997) to calculate the Hessian of the tangent linear model. Since the model under consideration is non-linear, it is crucial to compute the Hessian at the global minimum of the cost function, that is for the optimal parameter set. We ensure this by conducting the sensitivity analysis for identical twin experiments, where synthetically produced data are taken as observations. In this case, the optimal parameter set is known, since it was used to generate the synthetic data set.

3. Sensitivity experiments

The sensitivity analysis is based on identical twin experiments at the Bermuda station at 31°40′N 64°10′W, which is part of the U.S. JGOFS program. A synthetic data set was created by monthly sampling of the simulated model course from January 1989 to December 1992 (Fig. 2), using the initial

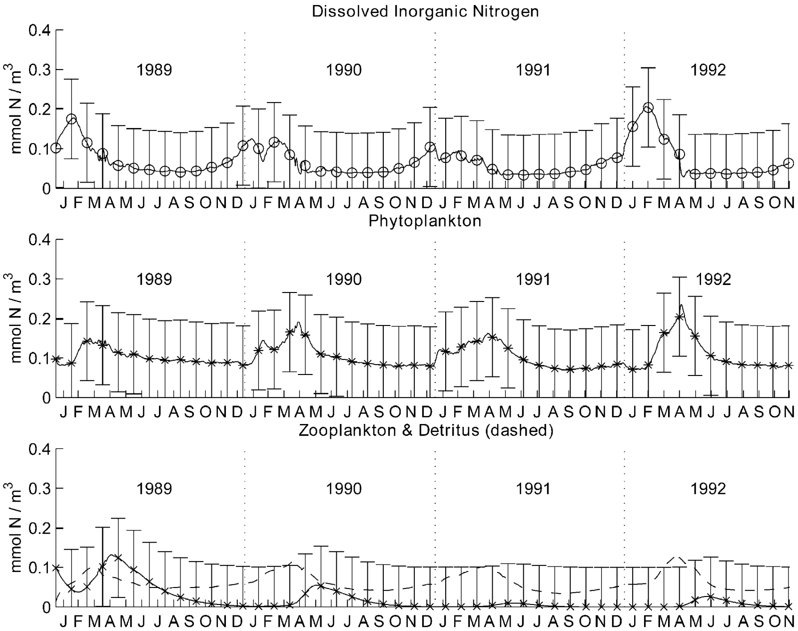


Fig. 2. Simulated model course at the Bermuda station. A synthetic data set was produced by monthly sampling (circles, asterisks and crosses represent the synthetic data). The errorbars represent the assumed a priori errors σ_i.

parameter values given in Table 1. The inverse formulation of the parameter estimation problem is obtained by defining the cost function

$$F(\vec{p}) = \frac{1}{2\sigma_{\mathrm{DIN}}^2}\sum_{i=1}^{M}\left(\mathrm{DIN}^{\mathrm{obs}} - \mathrm{DIN}^{\mathrm{sim}}\right)^2 + \frac{1}{2\sigma_{\mathrm{Phy}}^2}\sum_{i=1}^{M}\left(\mathrm{Phy}^{\mathrm{obs}} - \mathrm{Phy}^{\mathrm{sim}}\right)^2 \left(+\frac{1}{2\sigma_{\mathrm{Zoo}}^2}\sum_{i=1}^{M}\left(\mathrm{Zoo}^{\mathrm{obs}} - \mathrm{Zoo}^{\mathrm{sim}}\right)^2\right). \quad (11)$$

Please note that the third term on the right hand side of the equation accounts for zooplankton data and is only relevant for the experiments E4 and E7 (Table 2). The weights $1/\sigma_i^2$ are chosen to be equal for the dissolved inorganic nutrients, phytoplankton and zooplankton ($\sigma_i = 0.1$ mmol N m^{-3}, $i = $ DIN, Phy, Zoo). The Hessian of F is calculated according to the procedure described in Section 2.3.

3.1. Experiment E1—assimilation of nitrate and phytoplankton at the Bermuda station

For the first assimilation experiment (E1, Table 2) we employ monthly nitrate and phytoplankton data. This corresponds to the data availability from the Bermuda Atlantic Time-series Study (BATS). The Hessian matrix for this formulation was calculated. Its condition number is 9.0×10^7, indicating a nearly singular Hessian and an ill-conditioned problem formulation. The a posteriori errors (given in Table 3) are enormous especially for the initial slope of the PI-curve α, the fraction of photosynthetically active radiation par and the parameters related to zooplankton, that is the maximum grazing rate μ_{Z}, the half-saturation constant for ingestion k_{P} and the zooplankton mortality λ_{ZD}. The parameter resolution, given by the eigenvectors and eigenvalues of the Hessian, is shown in Fig. 3. The eigenvectors belonging to the smallest eigenvalues represent combinations of parameters that either cannot be determined at all or have large uncertainties. By far the smallest eigenvalue is $\lambda_1 = 1.4 \times 10^{-6}$. The corre-

Table 2
Description of the twin experiments E1–E8

Experiment	Comments
E1	Monthly nitrate and phytoplankton data at the BATS site were employed. All 12 biological model parameters are included in the inversion.
E2	Monthly nitrate and phytoplankton data at the BATS site were employed. par and the maximum grazing rate μ_Z were kept fixed.
E3	Monthly nitrate and phytoplankton data at the BATS site were employed. par, μ_Z and the maximum growth rate μ_P were kept fixed.
E4	Monthly nitrate, phytoplankton and zooplankton data at the BATS site were employed. par, μ_Z and μ_P were kept fixed.
E5	Monthly nitrate, phytoplankton and nitrate uptake data at the BATS site were employed. par, μ_Z and μ_P were kept fixed. (compare E3)
E6	Monthly nitrate and phytoplankton data at the North Atlantic site were employed. par and μ_Z were kept fixed. (in analogy to E2)
E7	Monthly nitrate, phytoplankton and zooplankton data at the North Atlantic site were employed. par and μ_Z were kept fixed.
E8	Monthly nitrate and phytoplankton data at the BATS and the North Atlantic sites were employed. par and μ_Z were kept fixed. (combination of E2 and E6)

sponding eigenvector $\vec{v}_1$ has significant contributions only for the light parameters α and par. Thus, all information on the independent component of α and par is represented by $\vec{v}_1$. As the corresponding eigenvalue λ_1 is extremely small, the independent component of α and par cannot be determined by assimilation of the data or, in other words, α and par cannot be determined independently. Inspection of the model equations reveals that α and par enter the model only in multiplicative combination (compare Eq. (3)). Thus, the indefiniteness of the combination of α and par results from the model formulation of the light-curve and the dependence of both parameters is not surprising. However, since α and par enter the model only in multiplicative combination, all we need to optimize is their product. By denoting $\hat{\alpha} := \alpha \cdot \text{par}$ we reformulate Eq. (3) to

$$F(I) = \frac{\hat{\alpha} I}{\sqrt{\mu_P^2 + \hat{\alpha}^2 I^2}}. \qquad (12)$$

In all following experiments, we restrict the optimization to the combination $\hat{\alpha}$. This is realized

Table 3
Condition numbers and a posteriori errors for experiments E1–E8

Exp.	E1	E2	E3	E4	E5	E6	E7	E8
Cond.	9.0×10^7	1.2×10^4	1.1×10^4	1.7×10^4	1.1×10^4	1.6×10^5	1.2×10^5	3.0×10^4
Post.								
μ_P	2.5	2.4	–	–	–	0.62	0.45	0.37
k_N	2.2	2.2	1.4	1.2	1.4	1.3	1.1	0.36
λ_{PD}	3.6	3.6	3.4	2.8	3.4	2.4	1.7	1.2
λ_{PN}	6.1	5.9	5.5	4.4	5.5	4.3	4.7	2.1
μ_Z	49	–	–	–	–	–	–	–
k_P	53	1.4	1.4	0.84	1.4	2.9	1.4	1.1
λ_{ZD}	12	10	10	3.7	10	3.4	1.2	1.8
λ_{ZN}	2.3	1.5	1.5	0.87	1.5	2.8	1.3	1.0
λ_{DN}	4.2	4.2	4	3.6	4.0	4.8	3	2.2
α	596	1.8	1.5	1.3	1.5	2.2	2.3	0.97
par	596	–	–	–	–	–	–	–
w_D	5.7	4.7	4.5	2.9	4.5	3.2	1.5	1.3

All errors are scaled by the initial parameter values.

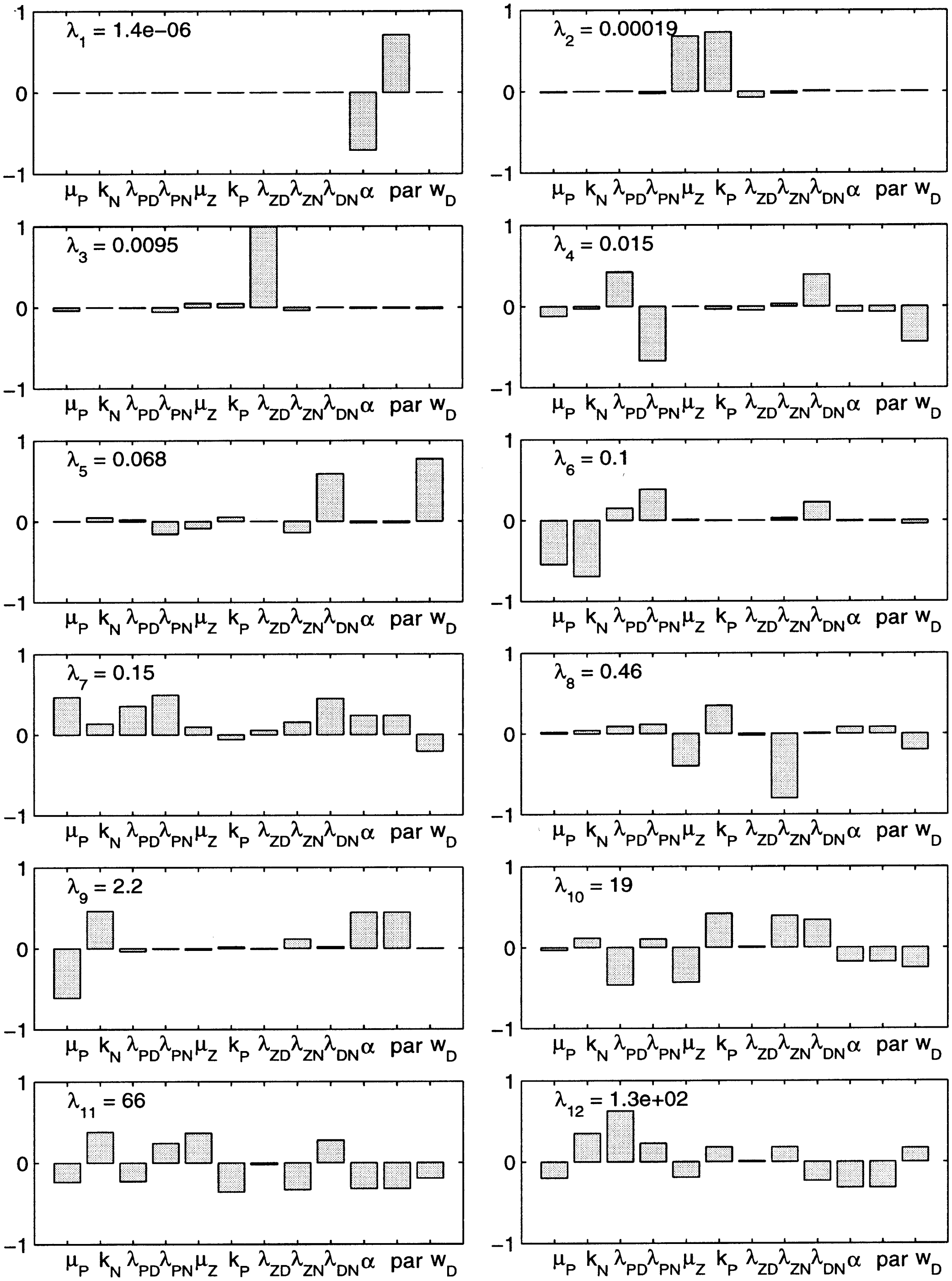


Fig. 3. Parameter resolution for experiment E1. Monthly measurements of nitrate and phytoplankton concentrations were employed.

practically by fixing par on the initial guess and seeking only α.

The second smallest eigenvalue is $\lambda_2 = 1.9 \times 10^{-4}$. The corresponding eigenvector $\vec{v}_2$ combines information on zooplankton parameters, basically the grazing parameters μ_Z (maximum grazing rate) and k_P (half-saturation constant for phytoplankton ingestion), with a small contribution from the zooplankton mortality λ_{ZD}. The combination of μ_Z and k_P is only poorly constrained by the data, or in other words their a posteriori errors are large. A possible reason might be that the simulated model course is almost stationary, that is, the state variables change only slightly with time. The phytoplankton standing stocks in the subtropical North Atlantic remain at a low and relatively constant level compared to regions with a more pronounced seasonal cycle, such as the midlatitudes of the North Atlantic, which are characterized by a strong increase of nutrient concentrations during deep winter mixing events and high plankton standing stocks during the typical spring and autumn blooms. In accordance with observations (Michaels and Knap, 1996), the simulated phytoplankton concentrations at the BATS station remain between 0.1 and 0.2 mmol N m^{-3} and the model course shows no high amplitude signals. Consequently, the grazing rates that correspond to the data cover only a small range of the parameter space close to the stationary point. In this case, the grazing rates that correspond to the "measured" data are limited to the initial slope of the grazing response. No data points lie within the saturation range (Fig. 4). The information contained in the data does not suffice to estimate both the half-saturation constant and the saturation rate at the same time. The same problem applies to the determination of the growth parameters μ_P (maximum growth rate) and k_N (half-saturation concentration for nitrate uptake). The simulated growth rates cover a slightly broader range than the grazing rates, but are still limited to the initial slope of the growth response (Fig. 4).

3.2. Experiments E2 and E3—a modification of the problem formulation

As a result of experiment E1, the maximum grazing rate and the half-saturation constant for phytoplankton ingestion cannot be estimated simultaneously. We believe this to be due to the fact that grazing rates are restricted to a small part of the grazing response function. Thus, the applied data set does not contain enough information to determine both parameters simultaneously. The same problem applies to the phytoplankton growth function where data are restricted to the initial slope of the growth response. The maximum growth rate and the half-saturation constant for nutrient uptake may not be estimated at the same time.

To test this hypothesis we check first if the conditioning of the problem improves when we restrict the search to the half-saturation concentrations and suppose we know the maximum grazing and maximum growth rates. In experiment E2 only the maximum grazing rate μ_Z was kept fixed at the optimal value. This modification improved the condition number considerably to 1.2×10^4. Also the a posteriori errors are smaller for most of the parameters (Table 3). In particular the errors of k_P and α are reduced by two and three orders of magnitude, respectively. In experiment E3, the maximum growth rate μ_P was held constant as well. This leads again to a small improvement of the condition number and the a posteriori errors. However, as the errors range from 140% for k_P to 1000% for the zooplankton mortality λ_{ZD}, they are still far from being acceptable.

The parameter resolution for E3 is shown in Fig. 5. Note that the first four eigenvectors that correspond to the smallest eigenvalues are very similar in experiments E2 and E3. The most uncertain parameter combination $\vec{v}_1$ contains information only on the mortality rate of zooplankton λ_{ZD} while contributions for λ_{ZD} are negligible in all other eigenvectors. Thus, λ_{ZD} is independent of the other parameters and practically not constrained by the data. This is consistent with the outstanding large a posteriori error of 1000% for λ_{ZD}. We assume that this is due to lack of data.

The schematic of the model state variables and flows (Fig. 1) illustrates that fluxes between phytoplankton, zooplankton and detritus are not directly constrained by the data set used. The model allows different pathways to close the nitrogen cycle, namely phytoplankton → zooplankton → detritus → nitrogen and phytoplankton → detritus → nitrogen. The recycling pathways are likely to be unconstrained if neither zooplankton nor detritus information is available. The conditioning of the problem might improve

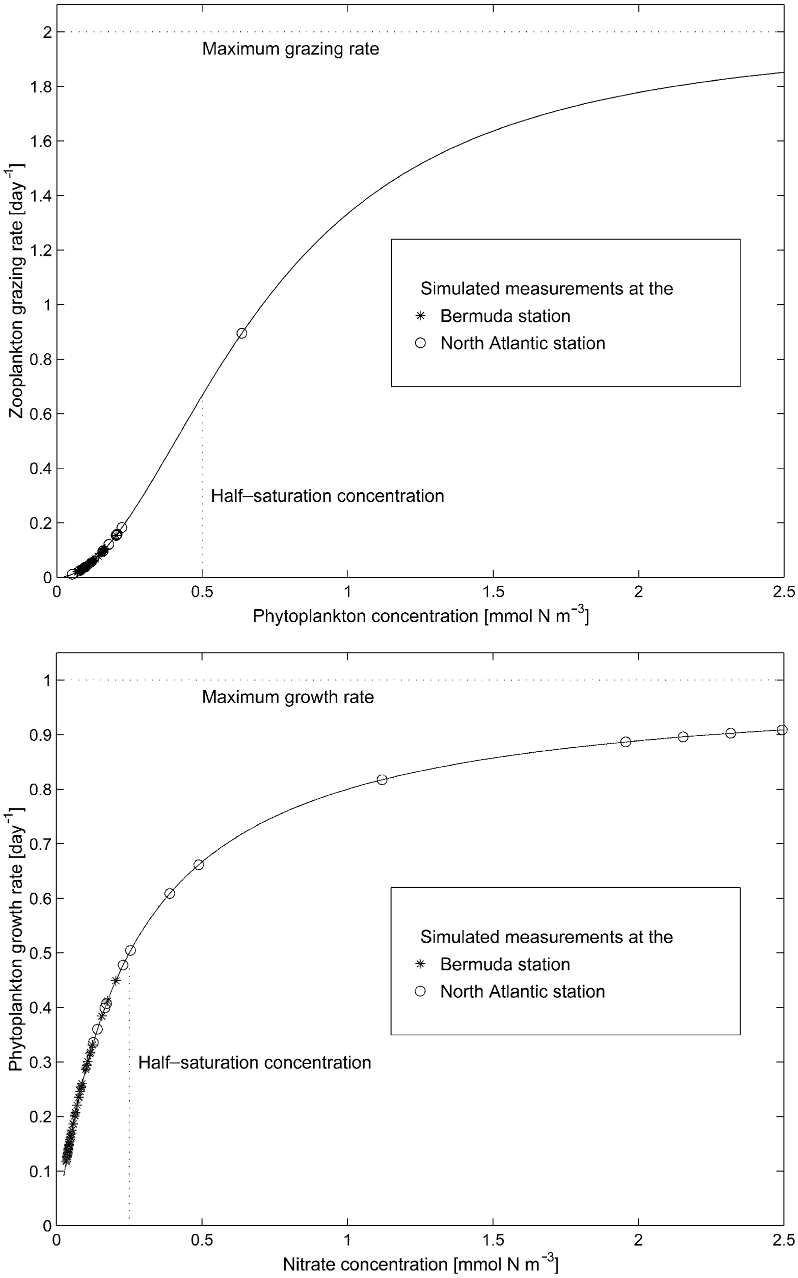


Fig. 4. Zooplankton grazing and phytoplankton growth response. Actual growth and grazing rates corresponding to the synthetic monthly data points are calculated as $\mu_P \frac{\mathrm{DIN}}{k_N + \mathrm{DIN}}$ and $\mu_Z \frac{\mathrm{Phy}^2}{k_P + \mathrm{Phy}^2}$, respectively. Values are displayed for the Bermuda station (asterisks) and a North Atlantic station (open circles), which we refer to in Section 3.4.

if other types of measurements, e.g. observations of zooplankton or fluxes, are incorporated. This consideration motivates the following experiments E4 and E5.

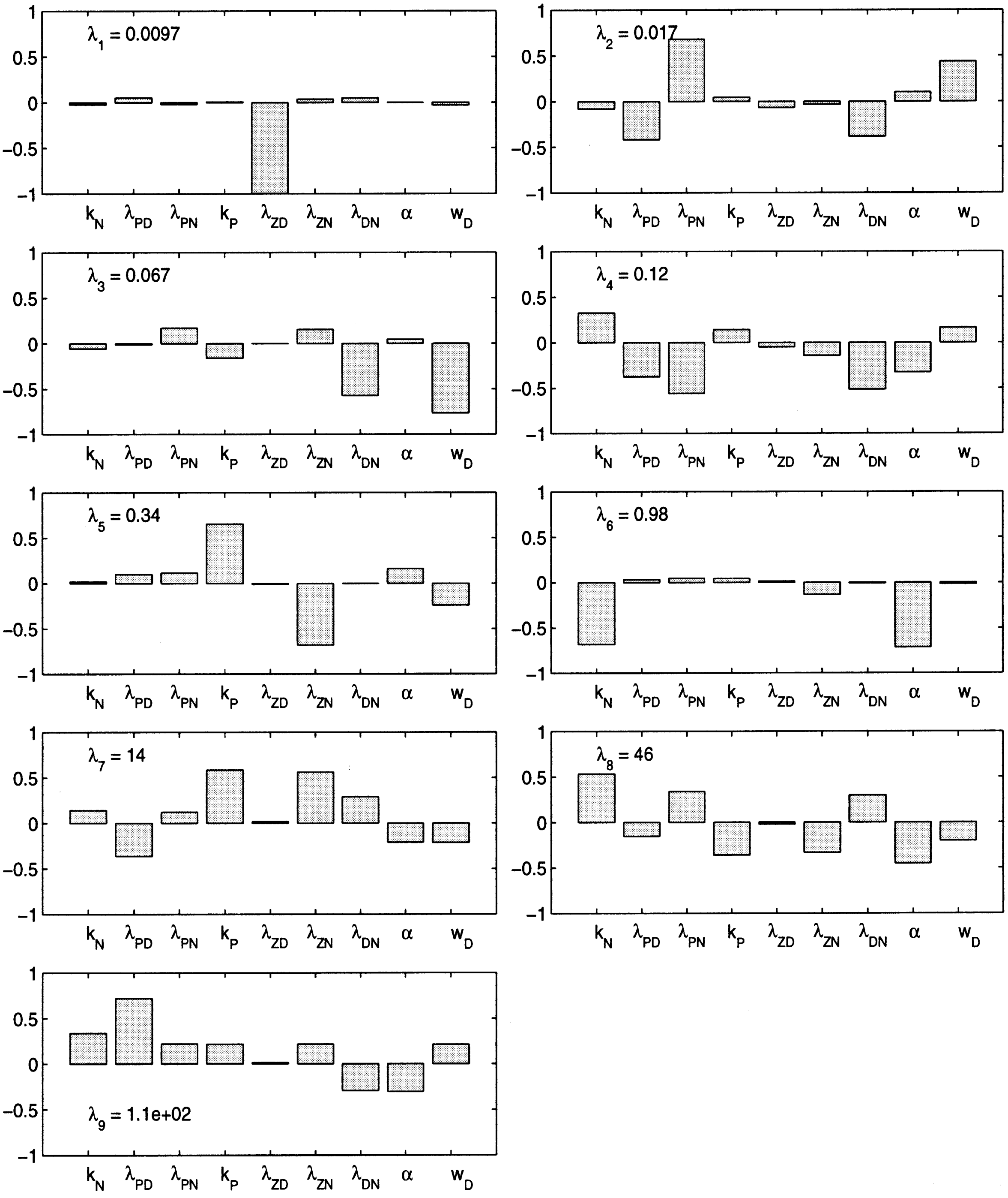


Fig. 5. Parameter resolution for experiment E3. Monthly measurements of nitrate and phytoplankton concentrations were employed. par, μ_Z and μ_P were kept fixed.

3.3. Experiments E4 and E5 — additional employment of zooplankton and primary production data

We suppose that the large a posteriori errors in experiment E3 are due to gaps in the employed data set, which comprises only nitrogen and phytoplankton data. In experiment E4, we modify E3 by the additional inclusion of zooplankton data. A remarkable increase in the accuracy of the estimated parameters is achieved by the incorporation of zooplankton data. The a posteriori errors improved in particular for the zooplankton related parameters k_{P}, λ_{ZN} and λ_{ZD}, but also for all the other parameters. Note that in spite of the decreased errors, the condition number of the Hessian is slightly larger than for E3. This means that the new data does not add information to the poorly determined combination of parameters which is represented by the smallest eigenvalue. Instead, the new data increase the precision of the already well determined parameter combinations. In terms of the Hessian spectrum, the largest eigenvalues are raised even further, thereby increasing the range of the spectrum.

Several parameter optimization studies employ measurements of primary production in addition to nitrate and chlorophyll data. Experiment E5 is performed to assess how this additional information affects the accuracy of the parameter estimation. Experiment E5 compares to E3, differing from E3 only in the inclusion of the actual nitrate uptake rate measurements, that is $g_{\mathrm{P}}\mathrm{Phy}$, which corresponds to the use of primary production data in parameter optimization assimilations. The inclusion of the uptake rate data did not improve the accuracy of the parameters. This result suggests that measurements of the flux of nitrogen from the inorganic nitrogen pool to phytoplankton does not add any information to the system that is not already contained in the inorganic nitrogen and phytoplankton data.

3.4. Experiments E6, E7 and E8 — assimilation at the North Atlantic station at 47°N 20°W

Here we come back to the previously mentioned problem that the ecosystem dynamics at the Bermuda site is nearly stationary with relatively low plankton standing stocks. We hypothesized in Section 3.2 that the restricted data coverage of the functional growth and grazing response contributes to the difficulty of the parameters optimization problem. Some evidence for this was shown by the improved parameter accuracy after assuming that the maximum growth and grazing rates were known. To perform another check of this hypothesis, we apply the optimization procedure to a station at a different location in the North Atlantic where a broader coverage of the functional growth and grazing responses is provided. A simulation at the North Atlantic station at 47°N 20°W was performed, employing the previously used parameter set. The model course at this site has a pronounced seasonal cycle with a high amplitude spring bloom (Fig. 6). The corresponding uptake and growth rates spread over a wider range of the parameter space than at BATS (Fig. 4). The phytoplankton growth rates seem to be satisfactorily covered while the grazing rates are still restricted to the initial slope.

In analogy to experiment E2 we perform experiment E6 at this station. Inspection of the Hessian reveals that the phytoplankton parameters and the zooplankton mortality are determined with higher accuracy in comparison to E2, while the accuracy slightly decreased for a few other parameters. An additional incorporation of zooplankton, done in E7, reduces these errors. We assume that the best estimate of the parameters can be expected if we employ

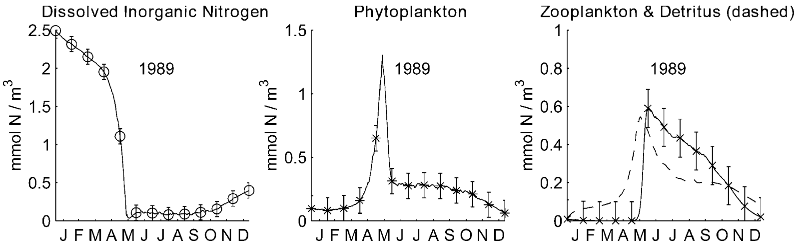


Fig. 6. Simulated model course at the North Atlantic station at 47°N 20°W and a synthetic data set that was produced by monthly sampling.

the North Atlantic and the Bermuda data sets simultaneously. This is done in E8. In E8 we achieved the best accuracy of all experiments. The most uncertain parameters with uncertainties of over 200% are the phytoplankton mortality λ_{PN} and the remineralization rate λ_{DN}.

4. Discussion of the sensitivity analysis

A sensitivity analysis was conducted to assess the capability of the adjoint method to optimize the ecological model parameters. The parameter optimization may be difficult for a variety of reasons. Generally, difficulties might be associated with the formulation of the inverse problem that is to be solved and with the numerical approach to its solution (Thacker, 1989). Difficulties might stem from the model formulation itself. The data may be another source of difficulty, i.e. they may be inadequate to determine the model parameters, thereby causing the least squares problem to be singular or ill-posed. By investigating the Hessian matrix of the problem we tried to sort out the different sources of difficulty. The initial formulation of the problem turned out to be ill-posed with parameter combinations that could be estimated only with large uncertainties and with expected slow convergence of the minimization algorithm. One difficulty obviously arose from the formulation of the model itself. Parameters that enter the numerical model formulation only as a product of each other cannot be estimated independently. In our first model formulation, the initial slope of the PI-curve α and the fraction of photosynthetically active radiation par occur as a product only. The uncertainty related to the unfavorable formulation can easily be circumvented by restricting the optimization to the combination of both parameters.

Furthermore, we found evidence that the information provided by the available measurements is not sufficient to constrain all parameters. Two major reasons cause the inadequacy of the data set. Firstly, the data set is restricted to only nitrate and phytoplankton observations. That turned out to be responsible for the poor accuracy of the parameters related to zooplankton behavior and the remineralization process, since two alternative unconstrained cycling pathways exist. Experiments with additional incorporation of zooplankton data displayed an improvement of the accuracy of these parameters. Secondly, it matters which region of the parameter space is covered by the data. Observations of an ecosystem which is close to equilibrium like at the Bermuda site provides less information on model parameters than ecosystems with pronounced seasonal changes. In particular the growth and grazing rates at the Bermuda site are restricted to the initial slope of the functional response and do not constrain the saturation concentrations. The inclusion of observations from a North Atlantic site with a clear yearly cycle provided a better coverage of the parameter space and increased the accuracy of the estimated parameters.

5. Parameter optimization at the Bermuda station

We performed a parameter optimization by assimilating data of the Bermuda Atlantic Time-series Study (BATS) (Michaels and Knap, 1996). Biweekly to monthly measurements of nitrate, nitrite and chlorophyll within the period January 1989 to October 1992 were employed. The observed data have been transformed as follows to serve as counterparts to the simulated variables. Nitrate and nitrite were added to be comparable to the dissolved inorganic nitrogen pool. Ammonium concentrations had to be neglected since ammonium concentrations are not measured on a regular basis. Chlorophyll measurements are generally assumed to represent the phytoplankton standing stock and were compared to the model phytoplankton. The necessary conversion from chlorophyll [mg chl m^{-3}] to phytoplankton [mmol N m^{-3}] is problematic, since the intracellular ratios of chlorophyll to carbon and chlorophyll to nitrogen are known to vary considerably. The chlorophyll to carbon ratio varies not only for different species but also due to changes in environmental conditions, e.g., differences in the ambient nutrient or light climate. Recently, different parameterizations for a variable chlorophyll to carbon ratio have been suggested in the context of parameter optimization (Hurtt and Armstrong, 1996, 1999; Schartau et al. 2000; Spitz et al. 2000) while other studies rely on a constant average conversion ratio (Evans, 1999;

Fasham and Evans, 1995; Prunet et al., 1996a,b; Spitz et al., 1998). We assume a constant ratio of $c_1 = 1.2$ mg chl (mmol N)$^{-1}$ in this study. The vertically distributed data were integrated over the prescribed mixed layer depth to correspond to the simulated mixed layer mean concentrations.

The sensitivity analysis discussed in Section 3 revealed that not all parameters can be determined by the optimization. Therefore, we restrict the inverse formulation to 8 of the 12 biological model parameters. The fraction of the photosynthetically active radiation par was fixed. An inclusion of par in the inversion is not appropriate since it enters the model formulation only in combination with the initial slope of the PI-curve α (see Section 3.1), but also not necessary since par is a relatively well known parameter. Furthermore, the maximum growth and grazing rates μ_P and μ_Z were excluded from the parameter estimation, since the nearly stationary ecosystem dynamics at the Bermuda station does not allow the optimization of the half-saturation concentrations and the corresponding maximum rates simultaneously (see Section 3.2). The twin experiments revealed that the zooplankton mortality rate λ_{ZD} is practically not constrained if only nitrate and phytoplankton observations are employed. Since no zooplankton data are available for our optimization problem, we also fixed the zooplankton mortality. par, μ_P, μ_Z and λ_{ZD} are fixed to the initial guess values (Table 1).

The cost function of the optimization problem has been defined as

$$F(\vec{p}) = \frac{1}{2\sigma_{\mathrm{DIN}}^2}\Sigma\left((\mathrm{NO}_3 + \mathrm{NO}_2)^{\mathrm{obs}} - \mathrm{DIN}^{\mathrm{sim}}\right)^2 + \frac{1}{2\sigma_{\mathrm{Phy}}^2}\Sigma\left(\mathrm{Chl}^{\mathrm{obs}}/c_1 - \mathrm{Phy}^{\mathrm{sim}}\right)^2 + F_{\mathrm{prior}}(\vec{p}) \qquad (13)$$

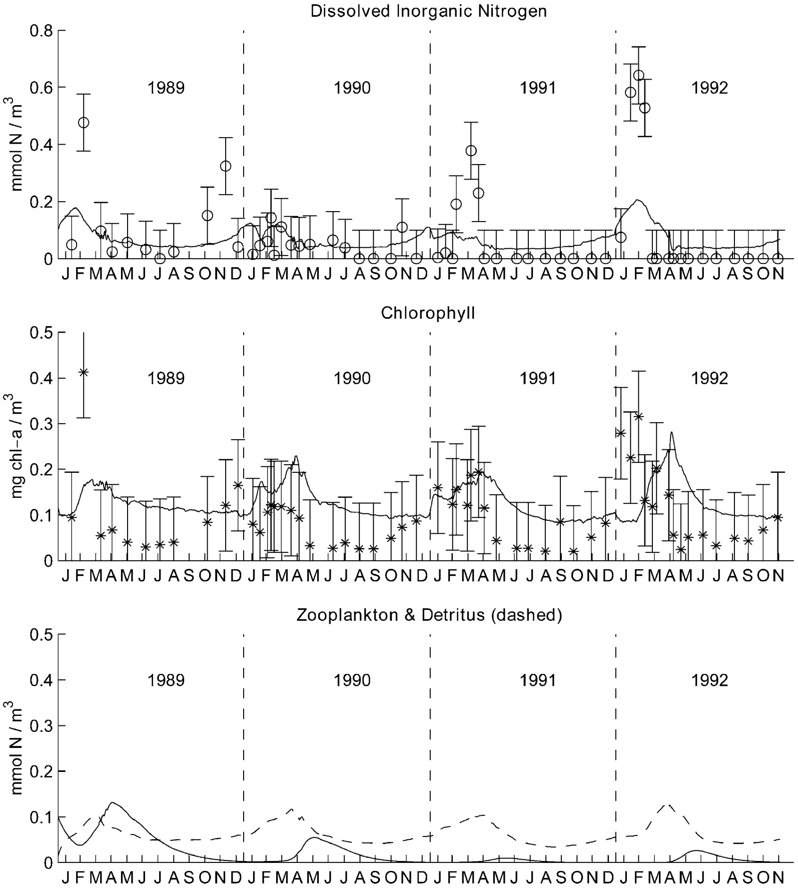
where $F_{\mathrm{prior}}(\vec{p}) = \frac{1}{2}\Sigma_i(\ln(p_i)/(p_i^0))^2$.

The first two terms of the right hand side of Eq. (13) represent the model-data misfit for the inorganic nitrogen pool and the phytoplankton standing stock respectively. The term F_{prior} was added to penalize estimates outside of the acceptable parameter range. As pointed out by Evensen et al. (1998), any available a priori information on the parameters should be used to constrain the problem. Unfortunately, we do not have much a priori information, but we know at least that negative parameter values are meaningless. Consequently we have chosen F_{prior} such that negative parameter values are avoided. Otherwise, negative parameter values might occur during gradient descent steps of the minimization algorithm. The variance σ_{DIN}^2 is based on estimated standard deviations of the measurements for nitrate ($\sigma_{\mathrm{NO}_3} = 0.08$ mmol N m^{-3}) and nitrite ($\sigma_{\mathrm{NO}_2} = 0.02$ mmol N m^{-3}) (Grasshoff et al., 1999). A standard deviation of $\sigma_{\mathrm{Phy}} = 0.1$ mmol N m^{-3} is assumed for phytoplankton measurements. Since the cost function in Eq. (14) differs from the cost function used for the twin experiments described above (Eq. (11) in Section 3), the error estimates for the twin experiments cannot be compared directly to the estimates for the real data experiment in this section. We have performed an additional twin experiment in analogy to Section 3 employing the cost function (14) to obtain the error estimates that directly correspond to the estimated errors for the real data experiment.

5.1. Results of the optimization

Our first guess for the model parameters is the previously used parameter set (compare Tables 1 and 4), which is based on parameter values in common use. The model simulation based on the first guess parameter set leads to relatively good agreement between the simulated course and the observed inorganic nitrogen and chlorophyll data (Fig. 7). The simulated course lies within the error range for most of the measurements. There are mainly three observed features that are not reproduced by the model. The model does not capture the increased nitrogen concentrations during the deep mixing periods in winter, especially in January, February and March 1992. The simulated chlorophyll concentrations are systematically higher than the observations during summer, and the simultaneous increase of observed chlorophyll concentrations and inorganic nitrogen from late autumn to early winter is not captured by the model.

The optimized parameter values with their a posteriori error estimates and the a posteriori errors for


Dissolved Inorganic Nitrogen

Chlorophyll

Zooplankton & Detritus (dashed)

Fig. 7. Simulated model course (solid and dashed lines) at the Bermuda station based on the initial guess parameter set in comparison to the observed data (circles/asterisks) with a priori error bars.

the twin experiment are given in Table 4. The optimization changed the half-saturation concentration for nitrate uptake k_N and the phytoplankton respiration rate λ_{PN} most notably, with a decrease in k_N by

Table 4
Model parameters: initial guess, optimal estimate with absolute a posteriori errors and relative a posteriori errors (scaled by the optimal estimate), also shown are the relative errors of the corresponding twin experiment

Parameter	Initial value	Relative error	Optimal estimate with absolute errors	Relative error of twin experiments
k_N	0.25	0.81	0.043 ± 0.035 mmol N m^{-3}	0.55
λ_{PD}	0.05	0.65	0.084 ± 0.055 day^{-1}	0.50
λ_{PN}	0.05	0.58	0.116 ± 0.065 day^{-1}	0.81
k_P	0.5	0.54	0.275 ± 0.145 $(mmol\ N)^2\ m^{-6}$	0.63
λ_{ZN}	0.05	0.42	0.036 ± 0.015 day^{-1}	0.65
λ_{DN}	0.05	0.61	0.089 ± 0.055 day^{-1}	0.81
α	0.025	0.27	0.025 ± 0.007 $(W\ m^{-2})^{-1}\ day^{-1}$	0.27
w_D	1.0	0.28	0.97 ± 0.27 m day^{-1}	0.28

a factor of 5 and an increase in λ_{PN} by a factor of 2. The other parameters differ by about 50% or less from their initial guess. The model course, resulting from the optimal estimate, is shown in Fig. 8. Only a slight improvement of the match between observations and simulation is evident. The increase of inorganic nitrogen during the mixing event in January–February 1992 is more pronounced in the optimized simulation. The mismatch between model and data during summer periods improved slightly. The most obvious change between the initial and the optimized simulations is a dramatic increase in zooplankton concentrations, which are not constrained by any data.

An assessment of the a posteriori errors was done by calculating the Hessian matrix of the tangent linear model for the optimal parameter set according to Section 2.3. The resulting condition number of the problem is 435. This relatively small value indicates that the problem with prior knowledge term is well conditioned. The condition number of the corresponding twin experiment is small as well with a value of 106. The significant reduction of the condition number compared to Section 3 is due to the prior knowledge term F_{prior}, which obviously regularizes the problem. The prior knowledge also reduces the a posteriori errors (compare errors in Table 4 with previous results given in Table 3), but most errors still range around 50% of the initial parameter value. Note that most of the optimized values differ from their initial guess by less than their a posteriori error estimate.

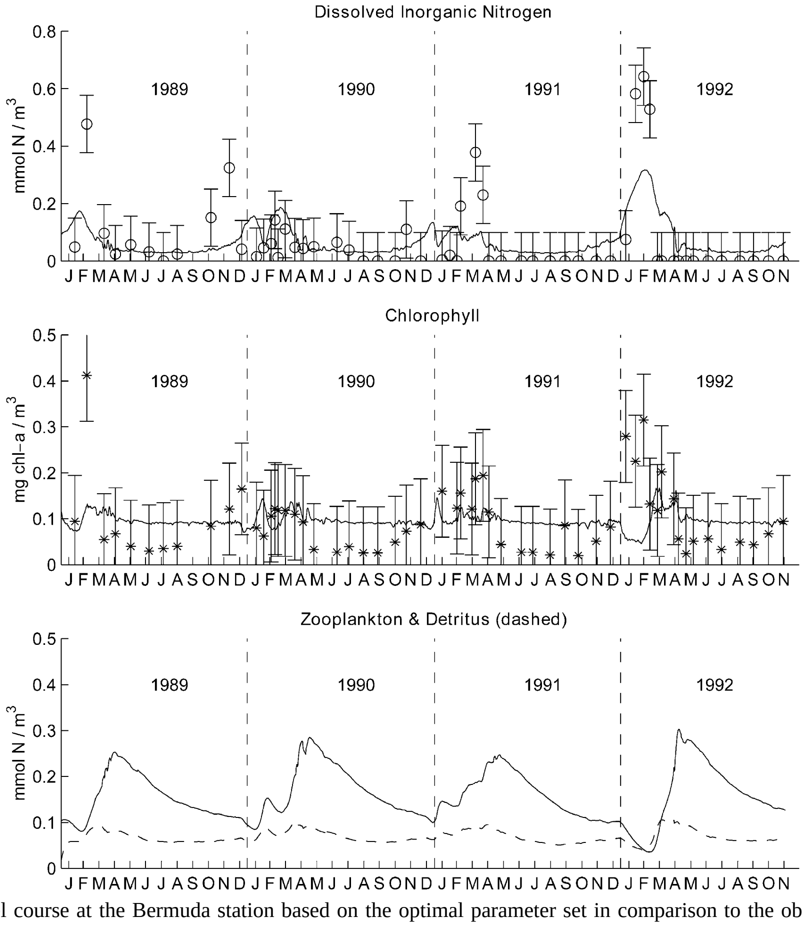


Fig. 8. Simulated model course at the Bermuda station based on the optimal parameter set in comparison to the observed data.

6. Discussion of the parameter optimization

The parameter optimization did not improve the match between the model and the observations notably. The simulation that is based on the new parameter set is very similar to the initial simulation in terms of nitrate and phytoplankton, which were constrained by observed data. The most obvious reduction of the model-data misfit was achieved for nitrogen concentrations during a deep mixing event in January–March 1992. The zooplankton course, which was not constrained by any observations, changed remarkably. This is consistent with the large uncertainties of the zooplankton parameters given by the sensitivity analysis, since large uncertainties of parameters allow large variations of these parameters during the optimization procedure.

There may be different reasons for the poor result of the optimization. Firstly, the course of the ecological variables depends largely on the physical forcing conditions, namely the mixed layer depth, which were prescribed. In terms of the parameter estimation procedure, prescribing the physical forcing is equivalent to the assumption that the forcing is correct. Thus, the optimization parameters are adjusted in such a way that they correct for any errors related to physical forcing conditions that influence the ecological state variables. Secondly, the model is zero-dimensional, which is clearly an oversimplification. All the ecological state variables are considered as average concentrations over the mixed layer. This misconstrues important features of the ecosystem at Bermuda, e.g. the deep chlorophyll maximum persistent below the mixed layer. A third potential reason for errors is the omission of advective transport processes in the model. Since mesoscale eddies influence the Bermuda region, advection is likely to be important.

However, a major concern goes beyond the issues related to spatial resolution and external forcing. The whole optimization has to be questioned if the model does not represent the observed system appropriately. The parameter optimization is bound to fail if the model does not resolve the processes which determine the observed features. The application of the optimization procedure to a specific model and a corresponding set of observations relies on the inherent assumption that the simulated and observed systems are consistent. The simultaneous increase of the observed chlorophyll and nitrate concentrations during deep mixing periods in winter is an example of such an unresolved feature, which is not possible to grasp with the present model formulation. It might be related to variations in the chlorophyll to nitrate ratio that are not resolved by the present model. Furthermore, the microbial loop, which is not included in the present model that is rather designed as a representation of the linear food chain, is probably an important factor.

7. Conclusions

A sensitivity analysis should be an integral part of any attempt to optimize the parameters of ecological models. Sensitivity experiments are extremely helpful in revealing problems that contribute to the difficulty of parameter optimization and formulation of a well-conditioned problem. There are sources of error related to an inappropriate formulation of the problem that can be circumvented. Furthermore, the sensitivity experiments can identify gaps or inadequacies in the applied data set. A data set can be insufficient because information on certain parts of the model is missing or because of poor coverage of the parameter space. In this context the sensitivity analysis goes beyond the rather technical issue of formulating the optimization problem as it provides feedback to observationalists about how to design field campaigns and sampling strategies that allow one to constrain numerical models.

The application of the optimization procedure to real data at the Bermuda station brought up a more fundamental problem. The parameter estimation gave poor results that we believe to be due to an inconsistency of the present model formulation with the ecological system under observation. This outcome emphasizes the important role that parameter optimization methods can play in testing model assumptions during model development. Since it is not possible to verify the theoretical assumptions underlying a model in principle (Oreskes et al., 1994) and, moreover, ecological modeling is mostly heuristic and in a comparably premature state, the model development has to be viewed as an iterative process where the refutation of model assumptions leads to the development of new hypothesies (Loehle, 1983). In this respect, the systematic test of parameter choices by the application of optimization techniques can be extremely powerful.

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