

# Sequential weak constraint parameter estimation in an ecosystem model

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## Abstract

A Sequential Importance Resampling filter is applied to assimilate data of the Bermuda Atlantic Time-series Study for the period December 1988 to January 1994 into a 9-compartments ecosystem model. The filter provides an opportunity to combine state and parameter estimations. We detected notable seasonality of some model parameters. A filtered solution is in close agreement with the data and is superior to that obtained with fixed model parameters. The seasonal dependence of the initial slope of the P-I curve agrees with other known estimates. The seasonality of the phytoplankton specific mortality rate obtained can point out that either the phytoplankton mortality parameterization has to be improved or the Chl:C ratio varies in time. Being of the same computational cost as the Ensemble Kalman filter, the data assimilation approach used can be implemented for on-line tuning and operational prediction the ecosystem dynamics with a coupled

## 1 Introduction

The skill of the prediction of the marine ecosystem dynamics depends crucially on reliability of model parameterizations of biological processes. They involve a number of parameters which are *a priori* poorly known. Estimating them from indirect observations has been attracted much attention (Fasham and Evens, 1995; Matear, 1995; Harmon and Challenor, 1996; Prunet et al., 1996; Hurtt and Armstrong, 1996; Spitz et al., 1996; Fennel et al., 2001; Schartau et al., 2001). Because of computational burden, it is not feasible to perform parameter optimization in the frame of a coupled hydrodynamical-ecosystem model for a sufficiently long period of integration. Instead the ecosystem was treated locally and the advection of biological compartments was neglected. In addition, it is worth to keep in mind that any model is an approximation to the real world and this is especially true for the ecosystem models which are not always derived from first principles of the nature. Consequently, the applicability of strong constraint data assimilation employed in all these studies becomes open to questions.

Kagan et al. (1997) and Natvik et al. (2001) attempted to account for model errors in ecological data assimilation. In both studies, model equations were imposed as weak constraints and a cost function was optimized by the conjugate gradient descent. These studies were

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concentrated on estimating the state of the ecosystem that is of our primary interest rather than the model parameters that play the role of auxiliary variables that were kept fixed. However, as it was demonstrated in Kagan et al. (1997) this procedure might fail when wrong parameter values were specified. Losa *et al.* (2002) proposed an extension of the method to tune the model parameters with accounting for model errors. They demonstrated that the ecosystem model parameters possess notable spatial variations. As such, it is difficult if not impossible to find a unique model parameter set which would be estimated locally and then used successfully in large-scale applications. The other conclusion was that the model errors make notable contribution to the solution and cannot be neglected. Thus, we need to seek for a data assimilation method for the ecosystem models that would account for the model errors, be applicable in the 3D context and be capable to optimise the model parameters.

Among approaches utilized in oceanographic data assimilation, sequential filtering methods meet the first two requirements. Until now, they have been successfully used for state estimation in ocean circulation models. Application of sequential data assimilation has been recently extended to the 1-D ecosystem model (Eknes and Evensen, 2001) and to coupled hydrodynamical-biogeochemical models (Natvik and Evensen, 2001; Carmillet et al., 2001). However, these studies were still concentrated on the state estimation and kept the model parameters fixed. Neglecting uncertainties in specification of the model parameters may result in overestimating the forecast skill and thus in underestimating the data contribution to the analysis.

Another point of trouble can be using the Kalman filtering or, in other words, the least square technique that can be extremely inefficient when dealing with "highly intermittent processes, such as fronts and blooms, having probability distributions not well characterized

by means and variances” (Bennett, 1992). The particle filters are free from these drawbacks. In a recent paper Kivman (2001) demonstrated that they make it also possible to optimize the model parameters sequentially and seemingly offer a data assimilation scheme that would serve all our needs. In that study, an extension of the Sequential Importance Resampling filter (SIR) was applied to optimization of some parameters of the stochastic Lorenz system and showed its high skills, at least, in deriving most crucial model parameters.

We employ here a modification of this approach to a more sophisticated 9-compartment ecosystem model and investigate its performance with the real-life BATS data. Our goal is twofold. At first, we show that one can benefit from simultaneous parameter and state estimation and obtain better fit to the data compared to that obtained with a fixed set of the model parameters. At second, the sequential technique used allowed us to study temporal variability of some model parameters, the issue that has not been examined yet in the ecosystem data assimilation. They may depend as on physical conditions (the temperature and light level) as chemical or biological characteristics (such as nutrient availability, optical properties of phytoplankton, phytoplankton species composition etc.). For example, it is well known that the slope of the P-I curve exhibits significant seasonal variations (Platt *et al.*, 1988). In all previous studies devoted to optimizing the ecosystem model parameters the cost function measuring the misfit between the system state and the data was defined globally over the whole assimilation period and the model parameters were assumed to be constants in time. However, it may turn out that a particular value of some model parameter is a good choice for one subperiod and is bad for another. With the sequential statistical methods, the cost function is defined locally for time steps when the observations are made. Hence, they seemingly offer a tool to let the data choose which set of the model parameters is the best

for each specific time step. Then looking at the history of the best estimates for the model parameters we can infer about parameter variability.

The paper is organized as follows. A description of a version of the filter used in the study is presented in the next section. In Sect. 3 we describe the design of a data assimilation experiment. Sect. 4 is devoted to numerical results of the experiment and Sect. 5 contains a discussion. Conclusions are presented in Sect. 6.

## 2 Sequential Importance Resampling filter for a parameter estimation problem

Predicting the evolution of a natural phenomenon with a dynamical model

$$\frac{d\mathbf{x}}{dt} = \mathbf{M}(\mathbf{p}, \mathbf{x}, t) + \mathbf{F}(t), \quad (1)$$

we have to keep in mind that neither prediction can be made with certainty. Generally, we are uncertain about all model inputs such as the initial condition  $\mathbf{x}(0)$ , true value of the internal model parameters  $\mathbf{p}$  and external forcing  $F$ , let alone the fact that each model is only an approximation (sometimes, a very crude one) to the truth. As such, the most general way to express the forecast is to output a probability density function (PDF) defined over a set of probable predictions.

This PDF  $\rho_t(\mathbf{x}(t), \mathbf{p})$  being defined on a joint space  $X_t \times P$  of the model variables  $\mathbf{x}(t) \in X_t$  and the admissible model parameters  $\mathbf{p} \in P$  can be expressed as

$$\rho_t^f(\mathbf{x}(t), \mathbf{p}) = C \rho^f(\mathbf{x}(t) | \mathbf{x}(0), \mathbf{p}) \rho_p(\mathbf{p}) \rho_0(\mathbf{x}(0)), \quad (2)$$

where  $C$  is a normalization constant, and  $\rho_p, \rho_0$  describes uncertainties in specification of the internal model parameters and in the initial condition. The conditional PDF  $\rho(\mathbf{x}(t)|\mathbf{x}(0), \mathbf{p})$  evolves in time according to the Fokker-Plank-Kolmogorov (FPK) equation corresponding to the stochastic dynamical system

$$\frac{d\mathbf{x}}{dt} = \mathbf{M}(\mathbf{p}, \mathbf{x}, t) + \mathbf{F}(t) + \varepsilon, \quad (3)$$

where  $\varepsilon$  is a stochastic process with the statistics describing the model errors. If for simplicity we consider a discrete analogue of the continuous system (3), then we can define a PDF globally over the space  $P \times X$ , where  $X = \Pi_t X_t$  is the space of the model trajectories,

$$\rho(\mathbf{x}, \mathbf{p}) = C \rho_p(\mathbf{p}) \rho_0(\mathbf{x}(0)) \prod_{k=1}^M \rho^f(\mathbf{x}(k\Delta t)|\mathbf{x}((k-1)\Delta t), \mathbf{p}) \quad (4)$$

where  $M$  is the number of time steps of the length  $\Delta t$ .

Availability of intermedient observations, which are also not perfect and contain some errors, makes it possible to reduce uncertainties in the forecast with use of the Bayes theorem. The detailed discussion of the Bayesian view on data assimilation can be found in van Leeuwen and Evensen (1996). In principle, Bayesian inference can be made globally over the space  $X \times P$ . However, it requires manipulations in the space of the dimension of  $M \dim(X_t) \dim(P)$  that makes the procedure impractical. Two simplifications are possible. In the most part of the studies dealing with data assimilation for ecosystem models, the dimension of the hypothesis space is reduced by neglecting the system noise  $\varepsilon$  that decreases the dimension of the problem to  $\dim(X_t) \dim(P)$ . This is the so-called strong constraint data assimilation.

Here we adopt another strategy and apply the Bayes theorem sequentially. That is, starting from  $t = 0$  we evolve the PDF  $\rho_t$  until  $t = t_1$  where the data  $\mathbf{d}_1$  become available. At  $t = t_1$ ,

we use  $\rho_t$  as the prior PDF and apply the Bayes theorem to get the analysis PDF

$$\rho_t^a(Vx(t_1), \mathbf{p} | \mathbf{d}_1) = C \rho_d(\mathbf{d}_1 | \mathbf{x}(t_1)) \rho_t^f(\mathbf{x}(t_1), \mathbf{p}), \quad (5)$$

describing updated knowledge about the system state and the model parameters. As one can see, while still accounting for uncertainties in the model equations the sequential data assimilation requires calculations in the space of the dimension of the same dimension as in the strong constraint case.

Being straightforward in the theory, the sequential data assimilation encounters a fundamental problem of evolving the forecast error statistics  $\rho_t^f$ . To solve this problem one needs to make a partitioning of the space  $X_t \times P$  and thus to solve the FKP for a domain of a large dimension even if  $\dim(X_t \times P)$  is of a moderate value. This problem can be easily overcome for the Gaussian statistics. In this case, instead solving the FKP to evolve the whole PDF one can evolve the corresponding covariance matrix that is much less costly. Though such a scheme referred to as the Kalman filter has been successfully used in oceanography for years (Ghil and Mallanotte-Rizzoli, 1991), strictly speaking, it works only for linear systems preserving the Gaussian shape of the initial PDF. In application to non-linear systems, one has to use a linearized FKP equation to propagate the error covariance matrix (the so-called Extended Kalman filter) and this linearization leads to several severe problems (see Evensen, 1994).

Monte Carlo methods offer a promising means to overcome them. The idea behind the methods of this type is approximating the continuous PDF with an ensemble of  $\delta$ -functions (particles) each of which evolves according to the stochastic dynamical model (3) and thus no linearization is involved. Any statistical moment of the forecast errors can be derived from this cloud of particles at any moment of time just by sampling. The strength of the Monte

Carlo methods is that their convergence rate does not depend on the space dimension. For example, the error in approximating an  $M$ -dimensional integral by with  $N$  regularly distributed nodes by the trapezium formula is  $O(N^{-2/M})$  while that for the Monte Carlo calculation is  $O(N^{-1/2})$ . The failure of the former method for high values of  $M$  is caused by the poor projection of the set of the nodes onto lower-dimensional subspaces while  $N$  randomly distributed nodes sample each dimension with exactly  $N$  species.

Monte Carlo methods enter the oceanographic data assimilation after Evensen (1994) who put forward the so-called Ensemble Kalman filter (EnKF). The EnKF uses the Monte Carlo technique for integrating the FPK equation to propagate the forecast error statistics. However, the analysis step (5) is still performed in the same way as in the Kalman filter, that is, using only the covariance matrix of the forecast error statistics. Kivman (2002) showed that this scheme could be extremely inefficient in application to strongly non-Gaussian distributions that is the case for the model parameters which are of constant sign.

In this study, we have utilized the Sequential Importance Resampling filter (SIR) introduced by Rubin (1988) and proposed for filtering dynamical systems in Gordon *et al.* (1993). In its simplest version, the SIR involves the following basic steps:

1. An initial ensemble  $\mathbf{x}_n, n = 1, \dots, N$  is drawn from a prior distribution  $\rho_0(\mathbf{x}(0))$ ;
2. Each ensemble member  $\mathbf{x}_n$  evolves according to the dynamical equations (3) with the noise  $\varepsilon$  produced by a random number generator according to the given statistics;
3. At  $t = t_k$  when the data  $\mathbf{d}_k$  become available, weights  $w_n(t_k)$  expressing "fitness" of ensemble members to the data are computed

$$w_n(t_k) = \rho_d(\mathbf{d}_k | \mathbf{x}_n(t_k))$$

and normalized so that

$$\sum_{n=1}^N w_n(t_k) = 1.$$

4. The ensemble of  $\mathbf{x}_n(t_k)$  is resampled with replacement with probabilities for each ensemble member to be drawn equal to normalized weights  $w_n(t_k)$ .
5. The analysis error statistics is approximated as

$$\rho_t^a(\mathbf{x}(t_k)) = N^{-1} \sum_{\alpha=1}^N \delta(\mathbf{x}(t_k) - \mathbf{x}_\alpha^r(t_k)), \quad (6)$$

where the superscript  $r$  denotes the resampled states.

6. The resampled ensemble  $\mathbf{x}_\alpha^r$  evolves till the next analysis step and the prediction is calculated as the ensemble mean

In principle, the 4-th step is not necessary and is done to improve the filter skill. One can update the weights recursively:

$$w_n(t_k) = \rho_d(\mathbf{d}_k | \mathbf{x}_n(t_k)) w_n(t_{k-1}),$$

and renormalize after each analysis step. Then the approximation to the analysis PDF instead of (6) is given by

$$\rho_t^a(\mathbf{x}(t_k)) = \sum_{n=1}^N w_n(t_k) \delta(\mathbf{x}(t_k) - \mathbf{x}_n(t_k)), \quad (7)$$

The scheme called the Direct Ensemble Method was tested in van Leeuwen and Evensen (1996). The authors reported a severe problem with the filter caused by effectively vanishing all but few weights  $w_n$  that resulted in a huge ensemble necessary to be used for obtaining a stable solution. The resampling step makes it possible to get rid of ensemble members deviating much from the data. Then, the system noise splits trajectories of those particles

resampled several times and allows one to achieve better coverage of the state space in the vicinity of the data values.

Similar to the EnKF, the SIR uses Monte Carlo integration to propagate the forecast error statistics. Contrary to the EnKF updating the ensemble states in the analysis step, the SIR updates probabilities of the ensemble members. This modification results in a fundamental difference between the filters. The SIR produces a discrete approximation of the analysis error statistics which tends to the true posterior probability density function with increasing the ensemble size (Smith and Gelfand, 1992). Thus, it is a truly variance minimizing scheme for any probability density function (PDF). This is just opposite to any Kalman filtering scheme applied to a non-linear dynamical system. At first, the Kalman filter employs only the Gaussian part of the forecast error statistics in the analysis step and thus is sub-optimal. At second, it has difficulties in propagating the error statistics in time. Even the EnKF that solves the FPK equation more accurately than the Extended Kalman filter is subject to this problem since it initializes the FPK equation with an ensemble drawn not from the analysis error statistics but from its Gaussian part.

In addition, there are some more benefits of using the SIR. At first, the analysis step is much simpler in the SIR than in the EnKF since no matrix inversion is involved. At second, since the SIR does not change the current state of the ensemble member and consequently no dynamical imbalance is introduced in the system at the analysis step. Finally, the filter can easily incorporate the data which are non-linearly related to the model variables.

An extension of the SIR for the parameter estimation problem is trivial. The ensemble should be drawn from the joint system state  $\times$  model parameter space. Then the set of the model

parameters remains fixed in time for each ensemble member while the dynamical components evolve according to the model equations with the corresponding model parameters until the analysis step. Here the ensemble member (and thus the corresponding set of the model parameters) may die if it deviates far from the data. Kivman (2002) demonstrated that the SIR was superior to the EnKF in estimating the parameters of the stochastic Lorenz system.

A potential problem with the SIR applied to the parameter estimation is that all but one parameter set die at the analysis step due to undersampling the parameter space or non-adequate representation of either the data or the model error statistics that are, in fact, not well known. If this is the case, the solution becomes very unstable and another initial ensemble will produce quite different results. A possibility to avoid the ensemble collapse is to add a noise to the resampled model parameters in order to split an ensemble member drawn several times onto several new particles. However, this procedure artificially extends the ensemble spread. Instead, after the resampling step we calculated the mean values of the model parameters and their variances and redrew the ensemble in the parameter space from a homogeneous distribution with the same first two moments. Of course, this is an *ad hoc* procedure which is difficult to be justified. However, we may consider the scheme adopted as a regularization of the problem of interest and refer to the inverse problem theory which is much older than data assimilation and where the suitable regularization still remains an active area of research.

### 3 Experiment design

The ecosystem model (see Fig. 1 for a schematic representation and Appendix for details) proposed by Drange (1996) was adopted in this study. Mainly, the model is built on the seven-compartment nitrogen-based model of Fasham *et al* (1990) (FDM-model). In order to simulate the carbon cycling within the upper mixed layer, dissolved and particulate organic carbon are added to the FDM-model. Thus, detritus and dissolved organic matter (DOM) are presented by carbon as well as nitrogen pools. Table 1 contains the list of 15 parameters to be optimized and while other model parameters kept fixed are listed in Table 2. The governing equations (8 - 15) were integrated in time with an explicit first order time-stepping scheme using the time step of 12 hours.

The model was constrained by the data of the Bermuda Atlantic Time-series Study (Michael and Knap, 1996), particularly, by measurements of nitrate, chlorophyll, particulate organic nitrogen (PON) and carbon (POC) concentrations for the period December 1988 to January 1994. For the data error variances we adopted the following values:  $0.05 \text{ mmolN/m}^{-3}$  for chlorophyll,  $0.1 \text{ mmolN/m}^{-3}$  for nitrate,  $0.1 \text{ mmolN/m}^{-3}$  for PON,  $1. \text{ mmolN/m}^{-3}$  for POC. All the data were averaged over the upper mixed layer (UML). The UML thickness was estimated by analyzing BATS temperature profiles. The UML depth was determined as the depth where the temperature is reduced by  $0.5^{\circ}\text{C}$  in comparison with the surface temperature (Fig.7). Nitrate concentrations at the upper boundary of the seasonal pycnocline were also estimated from the BATS data. To convert the phytoplankton biomass to the chlorophyll concentration we used the constant Chl:N ratio of  $1.2 \text{ mg Chl}(\text{mmol N})^{-1}$ .

Before starting the filter, one has to generate an initial ensemble of particles with the spread

reflecting uncertainties in knowledge of the initial state and the model parameters. The point is that usually we are provided with some first guess model parameter values obtained by trials-and-errors. Consequently, it is quite difficult, if ever possible, to establish a confidence interval for them. In this situation, it is obvious that overestimating the initial ensemble spread is less dangerous for performance of the SIR than underestimating. That was the reason for using the exponential distribution to generate the initial ensemble. This distribution maximizes the entropy and thus has the maximum uncertainty among all distribution localized at the non-negative semi-axis and having the same mean. That is, it is assumed that we know the initial system state and the model parameters with the relative standard error of 100%. In the parameter space, we take the first guess parameter values (Table 1) as the corresponding means. The mean initial system state was determined as the steady state solution to the model equations under the mean forcing averaged over the assimilation period. When generating randomly an initial ensemble, we assume that there is no correlations between initial values of the model compartments and the model parameters. To achieve stable results, we used a an ensemble of 1000 members.

We adopted a standard hypothesis that the model errors are described by a stationary Gaussian random process with zero mean and no correlations in time and between different noise components. The crucial factor affecting the filter performance is the variance of the system noise that is unknown *a priori*. If the noise is either too low, the trajectories of the particles resampled several times stay close to each other while, if it is too high, the ensemble spread will be too wide and the ensemble will tend to collapse due to large deviations of the vast majority of the ensemble members from the data. As a result, the solution will become unstable and will significantly change with changing the initialization of the

filter. The estimation of the model noise in the variational data assimilation is an area of active research and several recipes such as maximum likelihood (Cramer, 1954), the generalized cross-validation (Wahba, 1990), the L-curve method (Hansen, 1992) and the entropy maximization (Kivman *et al.*, 2001) have been put forward. Unfortunately, they cannot be applied directly in the frame of the statistical methods of data assimilation. Thus, we were forced to estimate the proper noise level that resulted in a stable solution simply by trial-and-errors. The variances adopted for the different components the model noise are approximately of about 20% of the characteristic value of the flux in the corresponding model equation.

## 4 Results

Fig.3 depicts the temporal evolution of the parameter estimates. We can reach stable estimates of  $g$  and  $\mu_4$  after few analysis steps. Seemingly, these parameters are amongst the most crucial model inputs and thus can be determined from the data with highest accuracy. After 3 years of the negative trend, the estimate for  $\mu_3$  also stabilizes. Another group of parameters ( $\mu_2$  and  $k_6$ ) exhibits fluctuations around the first guess. The behavior can be explained by either high quality of the first guess value or by tolerance of the solution to changes of these parameters. Analogous behavior is demonstrated by  $k_3$  with oscillations around a doubled first guess value. We can conclude that this parameter is recovered but the accuracy is rather low. Some parameters ( $\psi$  and  $w$ ) were notably disturbed initially and then they slowly relax to their optimal values.

The estimate for  $k_4$  remains rather stable until January 1993 when it dramatically increases

and then falls off in January 1994. It is worth noting that the estimates for  $k_2$  and  $k_6$  also exhibit the jump in January 1993 that is caused by a very high nitrate concentration observed while a very high value of the chlorophyll concentration measured in October 1994 yields the sharp drop in the estimates for  $k_4$  and  $\mu_2$ . The situation occurred in the autumn 1994 will be discussed below.

Final estimates for the model parameters mentioned above are presented in Table 3. Keeping in mind that the prior variance was equal to the first guess value, we can conclude that we achieved notable uncertainty reduction in specification of these model parameters (except  $k_3$  for which the initial error even grew). We could not obtain a stable estimate for  $V_b$ . A negative trend in the estimates depicted in Fig.3 is pronounced and possibly a stable estimate can be reached with enlarging the assimilation period.

The most interesting point is the notable seasonal variability of  $\alpha$ ,  $\mu_1$  and  $k_5$ . After removing the negative trend in the estimates for  $k_1$  and  $k_2$ , one can also see also the seasonality with the highest values in the autumn and the lowest ones during the spring bloom. It is well known that some of the parameters, for example, the initial slope of the P-I curve ( $\alpha$ ), have a seasonal variability (Platt *et al.*, 1988). Our estimates of the  $\alpha$  parameter (Fig. 4) are in a good qualitative agreement with those of Sathyendranath *et al.* (1995): in winter and spring values of the initial slope of P-I curve are higher than in other seasons. For 1992 a good quantitative agreement with the estimates of Sathyendranath *et al.* (1995) is achieved for the optimized parameter. During other years the estimates of  $\alpha$  are underestimated compared with Sathyendranath *et al.* (1995) but the seasonal variability of the parameter exhibits the same features. It is worth noting that Kyewalyanga *et al.* (1998) found positive correlations between nitrate (+nitrite) and  $\alpha$  that is also easily seen from comparison of Fig. 2 and Fig. 3.

On the other hand, we know nothing about seasonal variations of the other parameters ( $\mu_1$ ,  $k_1$ ,  $k_2$ ,  $k_5$ ). We leave this issue till the next section.

Though it is difficult to conclude about optimal values of some model parameters, the corresponding solution that is the quantity of our primary interest fits closely almost all available data (Fig. 5). This is not the case for the solution produced by the SIR with the first guess model parameters (Fig. 6). It notably underestimates particulate organic carbon and particulate organic nitrogen and overestimates the summer chlorophyll concentrations. The lack of PON and POC constraints the detrital breakdown rate  $\mu_4$  very well and that is the reason for obtaining this value with the very high accuracy after few analysis steps.

Advantages of simultaneous parameter and state estimation is especially pronounced if we compare the solutions with the bacteria data. These data were not assimilated in the model and were left for the verification. Adjusting the model parameters made the fit to the bacteria data much better than that for the fixed parameter set. As can be seen from Fig. 5, in spite of discrepancies between the data and simulated bacteria at separate moments, the solution reproduces the observed positive trend of the bacteria concentrations since January 1989 till the autumn 1991 quite well. This was achieved due to decreasing the bacterial excretion rate during this period.

It is rather difficult to verify other model components against observations. There are no data on dissolved organic matter and only few ammonium and zooplankton observations from ZOOSWAT cruises are available for periods 5-17 August of 1989 and from 23 March to 9 April of 1990 (Malone et al., 1993, Caron et al., 1995). Mean ammonium concentration was  $0.09 \text{ mmol N/m}^{-3}$  for the first period and  $0.11 \text{ mmol N/m}^{-3}$  for the second, that is an

agreement with our ammonium estimates. Zooplankton biomass observed during the cruises was smaller than  $0.1 \text{ mmol N/m}^{-3}$  (Caron et al., 1995). The filtered solution fits the data (see Fig. 5) everywhere except for an unprecedented increase of zooplankton biomass up to  $0.4 \text{ mmol N/m}^{-3}$  in November 1994 preceded by a jump observed in the phytoplankton biomass and POC.

The situation taken place in the autumn of 1994 is quite unusual for the assimilation period. Indeed, 1994 was the only year when the UML deepens in the autumn when the nitrate level is low. The filter immediately responds to the data by decreasing  $k_1$  and  $k_2$  to increase the primary production that resulted also rising DON and DOC. More weight is also given to a trajectory with much higher PON since POC and PON evolve almost coherently. As a result, the zooplankton gets much more food and exhibits a very sharp rise. An interesting point is that the SIR simultaneously decreases  $k_4$  and thus produces a much higher concentration of bacteria that perfectly fits the data (let us remind that the bacteria data were not assimilated).

## 5 Discussion

It is rather difficult to distinguish whether the notable seasonality in the best estimates obtained for  $\mu_1$ ,  $k_1$ ,  $k_2$ ,  $k_5$  is fact or artifact. It might be a consequence of using the constant carbon to chlorophyll ratio for phytoplankton to convert the phytoplankton biomass to the chlorophyll concentration. The ratio is known to depend on numerous factors (Geider et al., 1996; Hurt and Armstrong, 1996). Our previous experience (Losa et al., 2002) in using an expression for the  $Chl : C$  ratio and accounting for the dependence of the ratio on

temperature, irradiance and nitrate concentration (Cloern et al., 1995) showed that the  $Chl : C$  ratio possessed seasonal variability with lower summer values. The excessive value of the  $Chl : C$  ratio for phytoplankton in the summer yields overestimating the simulated chlorophyll concentration and causes some artificial increase of the phytoplankton maximum specific mortality rate and decrease of the primary production to reduce the phytoplankton concentration in order to fit the data.

On the other side, if using the constant  $Chl : C$  ratio we calculate the phytoplankton concentrations from the chlorophyll data in the right manner, then we have to admit that the model overestimate the phytoplankton between the blooms (see Fig.6) and thus it needs less production or/and more sinking. The seasonality in  $\mu_1, k_1, k_2, k_5$  employes both options and pushes the solution just in the direction of decreasing the phytoplankton. This may give clues to errors in the parameterization of the phytoplankton mortality and the primary production. The temporal variations of  $\mu_1$  and  $k_5$  try to compensate deficiencies of the parameterization of the phytoplankton mortality and suggest that the parameterization adopted underestimates the phytoplankton mortality for low phytoplankton concentrations and overestimates the mortality rate when they are high.

As in other studies (Spitz *et al.*, 1998; Schartau *et al.*, 2001), we have problems in reproducing the measured primary production (see Fig. 7). However, our fit to the data being of the same quality was attained without assimilating the primary production data while these data constrained the solutions obtained in the studies. One can notice from Fig. 7 that the SIR does a much better job for the second half of the assimilation period (1992-1994) than that for the first half (1989-1991). After the initial three years the seasonal variations of  $k_1$  and  $k_2$  become more pronounced. As a consequence, with the combined parameter-state

estimation we were able to produce significantly higher values of the primary production which fit the observation made during the spring blooms much better compared to the state estimation with the fixed model parameters. Thus, we can also conclude that the seasonality of  $k_1$  and  $k_2$  tries to compensate errors in the parameterization of the primary production.

## 6 Conclusions

We presented an approach to sequential model parameter estimation. It is based on the Sequential Importance Resampling filter and incorporates the information about the model and data errors together with uncertainties in the model parameters specification in a unique solution that approximately fits the dynamical model and the data. Due to its sequential nature, the method permits detecting temporal evolution of the model parameters. For the Bermuda station, it is shown that the annual variability of some model parameters can be remarkable. Seasonality of the initial slope of the P-I curve obtained is in quantitative agreement with other estimates while that of the  $\mu_1$ ,  $k_1$ ,  $k_2$  and  $k_5$  can be an artifact caused by either wrong interpretation of the chlorophyll data or by the inadequate parameterization of the phytoplankton mortality and the primary production. In the later case, permitting temporal variability of the model parameters we were able to compensate the lack of the primary production in the spring and the phytoplankton mortality in the rest of the year and thus to improve notably the fit to the data in comparison with the solution with the fixed model parameters. The superiority of the combined state-parameter estimation in comparison with the state estimation is especially pronounced if the solutions are verified against the bacteria data not assimilated into the model.

It is not a surprise that we were not able to obtain stable estimates for all model parameters. The fact that there are significant correlations between the model parameters and not all of them can be derived from the data with high accuracy was emphasized in previous studies (see, for example, Fennel et al., 2001). Either longer time series or denser and/or more accurate data sets are needed to improve the quality of the estimates. This means that the model solution is not very sensitive to the choice of these parameters. Thus, the forecast skill slightly depends on this kind of uncertainties and is mainly limited by uncertainties in the parameters having the most impact on the system trajectory. Kivman (2002) showed that the SIR was able to recover those parameters within low errors with an ensemble of a few hundred members and performed much better than the Ensemble Kalman filter without increasing the computational cost.

Comparison of the solution with the primary production data shows that, though adjusting the model parameters together with estimating the system state allows us to achieve much better fit to the data, there is still much room for improving the results. Assimilating these data could be of help. It is worth to remember that the primary production is non-linearly related to the model variables. Assimilating data of this kind is a severe problem for any scheme of the Kalman filtering while it is quite straightforward for the SIR and will be a subject of future research.

The seasonality of the model parameters together with their spatial variability and importance of accounting for the model errors what was demonstrated in Losa et al. (2002) drastically complicates tuning the ecosystem models. The approach presented provides a feasible and more flexible alternative to traditional Kalman filtering schemes for implementation of sequential assimilation of the data into coupled hydrodynamical-ecosystem models.

An issue that is important as from the theoretical viewpoint as for practical applications of the SIR is elaboration of a procedure of choosing the system noise that would be more rigorous than the trial-and-error method. In principle, nobody prevents us from including the system noise variance in the list of estimated parameters. This problem will be examined in a future study.

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## 7 Appendix: Model Equations

The model includes, as dependent variables, phytoplankton ( $P$ ), zooplankton ( $Z$ ), bacteria( $B$ ), nitrate( $Nn$ ), ammonium( $Nr$ ), detritus as particulate organic nitrogen ( $PON$ ) and carbon( $POC$ ), dissolved organic nitrogen ( $DON$ ) and carbon ( $DOC$ ). The model equations describing the processes of entrainment-detrainment at the lower upper mixed layer (UML) boundary, sinking of detritus with velocity  $w_g$ , and inner biological sources and sinks  $S_i$  can be written as

$$h \frac{dc_i}{dt} + q_i^{h-0} + \delta_{i6,7} w_g c_{6,7} - h S_i = 0, \quad (8)$$

where  $h$  is the UML thickness,  $c_1 = P$ ,  $c_2 = Z$ ,  $c_3 = B$ ,  $c_4 = Nn$ ,  $c_5 = Nr$ ,  $c_6 = PON$ ,  $c_7 = POC$ ,  $c_8 = DON$ ,  $c_9 = DOC$ ,  $q_i (i = 1, \dots, 9)$  are the turbulent fluxes at the lower UML boundary,  $\delta_{i6,7}$  is the Kroneker symbol,  $t$  is time.

The fluxes  $q_i$  are parameterized in terms of the entrainment velocity ( $w_e = \frac{dh}{dt}$ ) in the common way, i.e.

$$q_i^{h-0} = \begin{cases} w_e(c_i - c_i^*), & \text{if } w_e > 0, \\ 0, & \text{if } w_e \leq 0 \end{cases} \quad (9)$$

where  $c_i^*$  are the concentrations of the components at the upper boundary of the seasonal pycnocline. All  $c_i$  except  $c_4$  were taken as 0 while  $c_4$  was estimated from the BATS data.

Biological sources and sinks  $S_i$  are expressed as

$$S_i = \begin{cases} (1 - \gamma)PP - G_1 - De_1 & \text{if } i = 1, \\ \beta_1 G_1 + \beta_2 G_3 + \beta_3 G_6 - F_8 - De_2 & \text{if } i = 2, \\ U_8 + U_4 - G_3 - De_3 & \text{if } i = 3, \\ -JQ_1 P & \text{if } i = 4, \\ -JQ_2 P - U_4 + De_3 + \epsilon De_2 & \text{if } i = 5, \\ (1 - \beta_1)G_1 + (1 - \beta_2)G_3 - \beta_3 G_6 - De_6 + De_1 & \text{if } i = 6, \\ (1 - \beta_1)G_1 + (1 - \beta_2)G_3 R_B - \beta_3 G_7 - De_7 + De_1 R_P & \text{if } i = 7, \\ \gamma PP + \delta De_2 + De_6 - U_8 + F_8 & \text{if } i = 8, \\ \gamma PPR_P + \delta De_2 R_Z + De_7 - U_9 + F_9 & \text{if } i = 9, \end{cases} \quad (10)$$

where  $PP = JQP$  is the average daily phytoplankton growth rate,  $J$  is the light-limited growth rate,  $Q$  is a non-dimensional limiting factor,  $G_1$ ,  $G_3$ ,  $G_6$ ,  $G_7$  are grazing rates of the zooplankton on the phytoplankton, bacteria and detritus (nitrogen and carbon pools) respectively,  $\beta_1$ ,  $\beta_2$  and  $\beta_3$  are equivalent assimilation efficiencies,  $De_1$  is the rate of phyto-

plankton natural mortality,  $De_2$  is the rate of zooplankton losses due to excretion, natural mortality and grazing by predators,  $De_3$  is the bacterial excretion rate,  $De_6$ ,  $De_7$  are the rates of breakdown of detritus to the both pools of DOM,  $\epsilon$  and  $\delta$  are fractions of the total zooplankton losses transformed into ammonium and DOM respectively (the remaining part  $1 - \epsilon - \delta$  of zooplankton losses transforms into detritus which is considered to be instantly exported to the seasonal pycnocline),  $U_4$ ,  $U_8$  and  $U_9$  are the ammonium uptake and the uptake of DON and DOC by the bacteria,  $F_8$  and  $F_9$  are flows of the nitrogen and carbon to the dissolved organic pools due to excesses of the nitrogen or carbon in the zooplankton food,  $R_P$ ,  $R_Z$ ,  $R_B$  are the carbon to nitrogen ratios ( $C : N$ ) of the phytoplankton, zooplankton and bacteria respectively. Following Fasham (1993), functions  $J$ ,  $Q$ ,  $De_1$ ,  $De_2$ ,  $De_3$ ,  $De_6$  and  $De_7$  are given as

$$\begin{aligned}
 J &= \frac{2}{h} \int_0^\tau \int_0^h F \left[ \frac{V_p \alpha I}{(V_p^2 + \alpha^2 I^2)^{1/2}} \right] dz dt, \\
 Q &= Q_1 + Q_2 = \frac{N n \exp(-\psi N r)}{k_1 + N n} + \frac{N r}{k_2 + N r}, \\
 De_1 &= \frac{\mu_1 P^2}{k_5 + P}, \quad De_2 = \frac{\mu_2 Z^2}{k_6 + Z}, \quad De_3 = \mu_3 B, \quad De_{6,7} = \mu_4 POM,
 \end{aligned} \tag{11}$$

where  $V_p = V_p^* 1.066^{T_w}$  is the maximum phytoplankton growth rate,  $\alpha$  is the initial slope of the P-I curve,  $I$  is the photosynthetically active radiation (PAR),  $t$  is measured in days and is 0 at sunrise and  $\tau$  at noon,  $T_w$  is the water temperature,  $z$  is the vertical coordinate,  $k_1$ ,  $k_5$ ,  $k_6$ ,  $\mu_1$ ,  $\mu_2$ ,  $\mu_3$ ,  $V_p^*$  are model parameters. Zooplankton grazing rates  $G_1$ ,  $G_3$ ,  $G_6$  and  $G_7$  are described by the expression:

$$G_i = \frac{gr_{i(i)} Z c_i^2}{k_3(r_1 P + r_2 B + r_3 POM) + r_1 P^2 + r_2 B^2 + r_3 POM^2}, \quad i = 1, 3, 6, 7, \tag{12}$$

which is a multi-prey generalization of the Holling type III function. Here  $l(1) = 1, l(3) = 2, l(6) = l(7) = 3$ ,  $r_1, r_2$  and  $r_3$  are the weighted preferences for phytoplankton, bacteria and particulate organic matter,  $g$  and  $k_3$  are the maximum specific rate and the half-saturation constant for grazing. The flows  $F_8$  and  $F_9$  equal the following:

$$F_8 = \max(0, R_{Z,food} - R_Z) f_{Z,N}, \quad F_9 = \max(0, R_{Z,food} - R_Z) \frac{f_{Z,N}}{R_Z}, \quad (13)$$

where

$$R_{Z,food} = \frac{f_{Z,C}}{f_{Z,N}} = \frac{\beta_1 G_1 R_P + \beta_2 G_3 R_B + \beta_3 G_7}{\beta_1 G_1 + \beta_2 G_3 + \beta_3 G_6}. \quad (14)$$

Functions  $U_4, U_8$  and  $U_9$  are presented as

$$\begin{aligned} U_4 &= \min(Nr/\Delta t, \max(0, \eta)U), \\ U_8 &= U + \min(0, \eta)U, \\ U_9 &= UR_{DOM} + \min(0, Nr/\Delta t - \max(0, \eta)U)R_B, \end{aligned} \quad (15)$$

here  $U = V_b B_{DON}/(k_4 + DON + \min(Nr, \eta DON))$  is the Michaelis-Menten formulation of the bacterial uptake (FDM),  $\eta = \frac{R_{DOM}}{R_B} - 1$ ,  $V_p$  is the maximum bacterial uptake rate,  $k_4$  - the half-saturation coefficient for uptake,  $\frac{Nr}{\Delta t}$  is the amount of ammonium that is available to support the growth of bacteria over the time step  $\Delta t$ . The Redfield ratios for DOM as well as for POM are calculated with the given carbon and nitrogen fluxes, as described by the model equations.

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## Figure captions

Fig. 1. The schematic diagram of the ecosystem model.

Fig. 2. The UML thickness at the Bermuda station.

Fig. 3. The evolution of the estimates for the model parameters. Values are normalized with respect to the model parameter initial values.

Fig. 4. Seasonality of the initial slope of the  $P - I$  curve at the Bermuda station from January 1992 till January 1993. The curve is the result of the parameter estimation, the solid horizontal lines are estimates of Sathyendranath et al. (1995) with the standard deviation (dashes lines).

Fig. 5. The evolution of the ecosystem components at the Bermuda station obtained by the sequential weak constrained parameter estimation. Circles are the BATS data for nitrate, chlorophyll, bacteria, particulate organic nitrogen and carbon. The data for ammonium (circles) are from Malone et al. (1993).

Fig. 6. The same as Fig. 5 with the initial model parameters.

Fig. 7. The primary production for the combined parameter-state estimation (black curve) and for the state estimation with the fixed model parameters (gray curve). Circles represent the data.

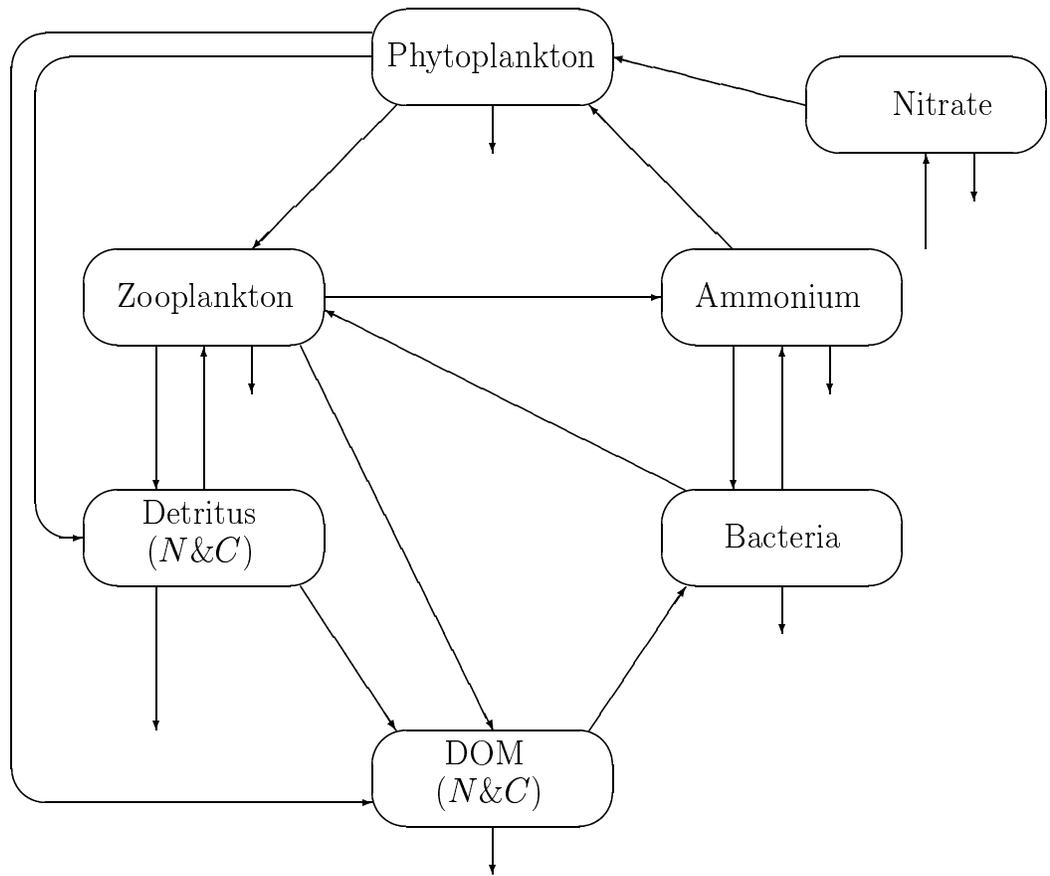


Fig. 1.  
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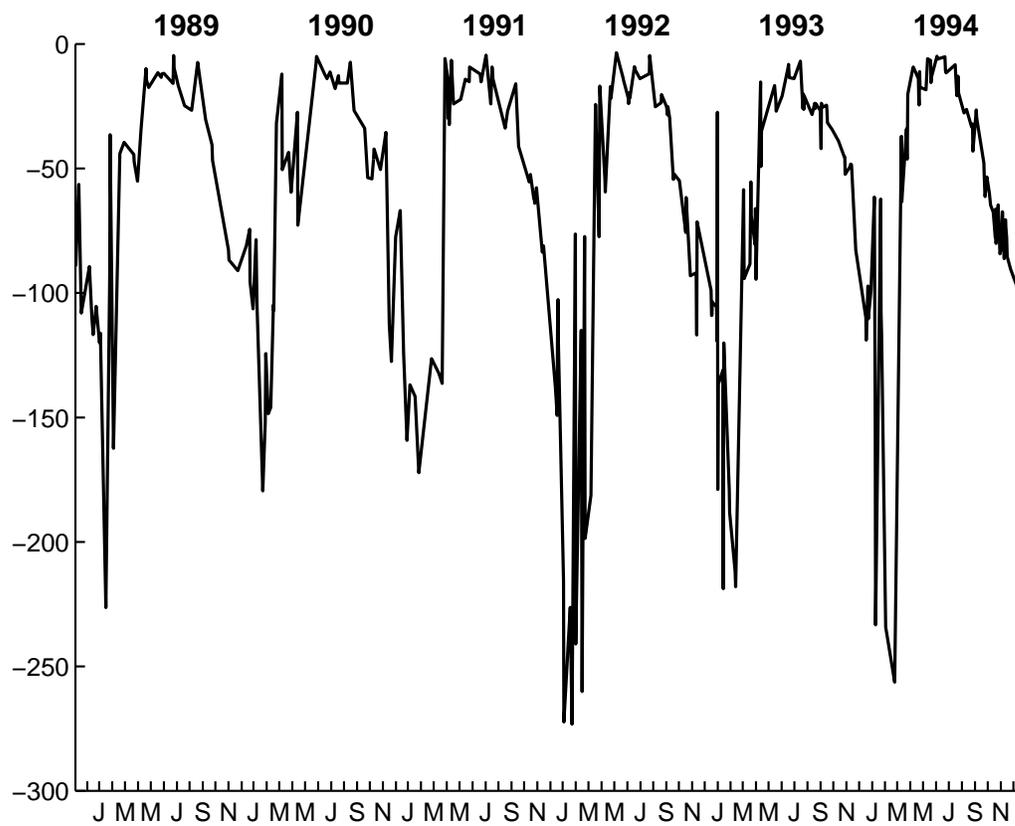


Fig. 2.

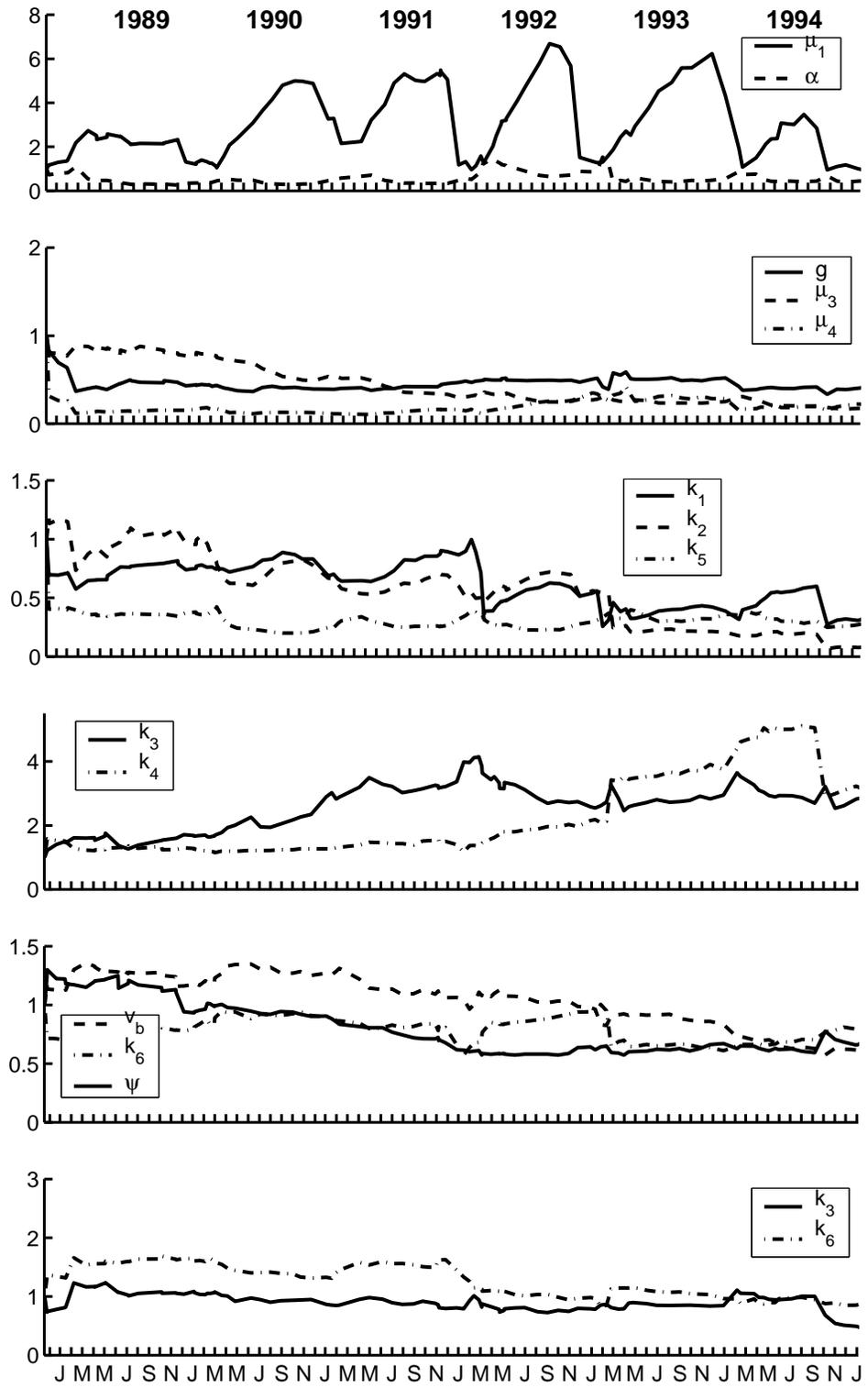


Fig. 3.

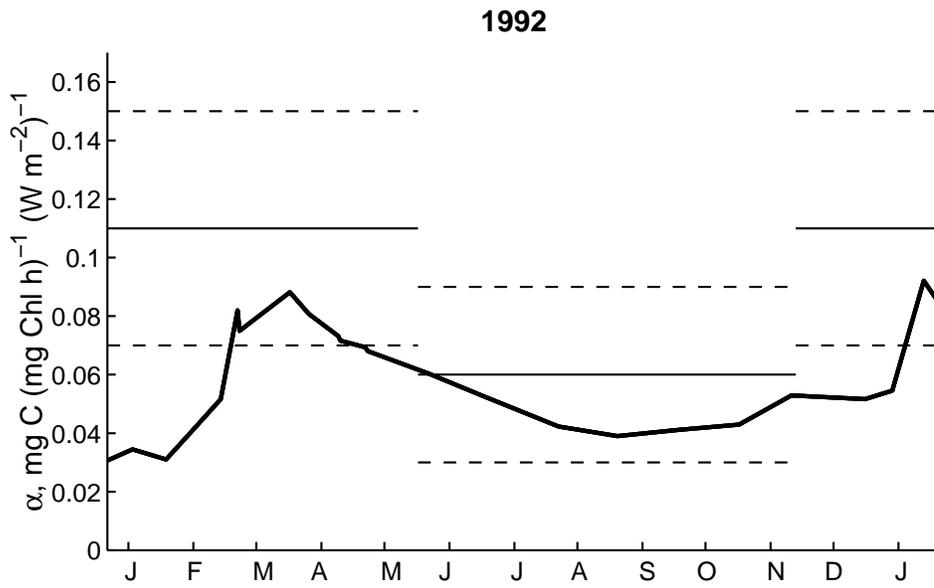


Fig. 4.

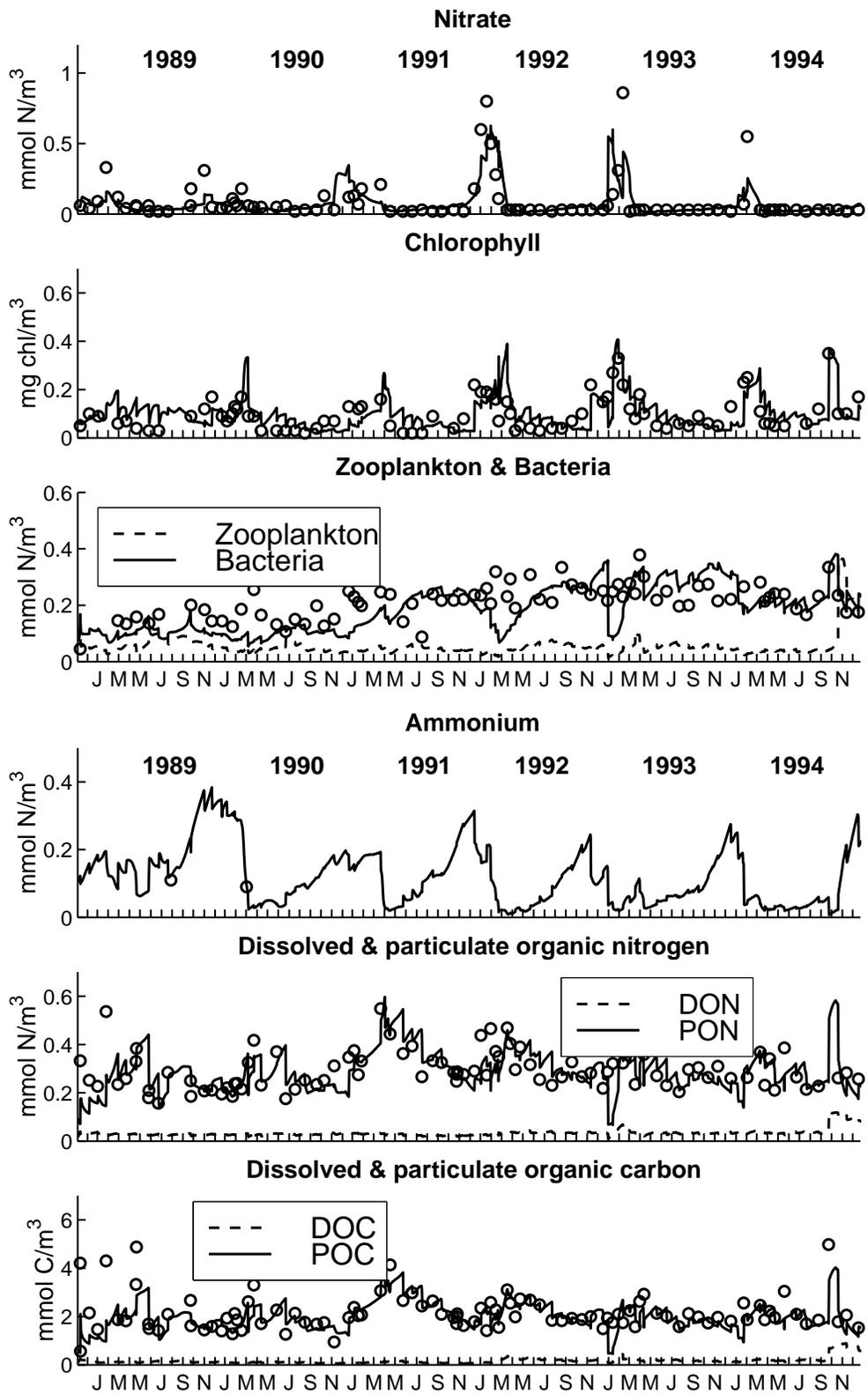


Fig. 5.

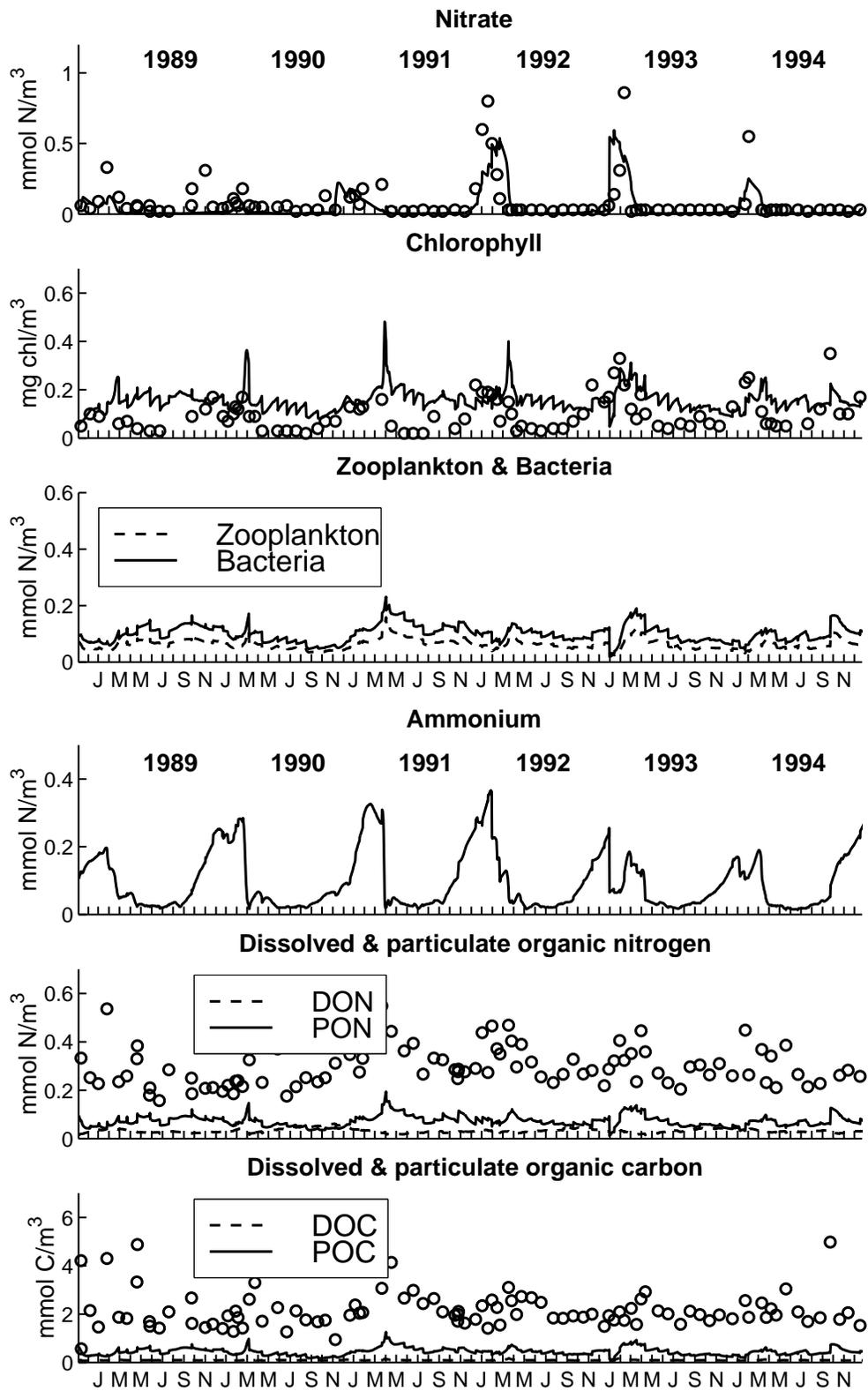


Fig. 6.

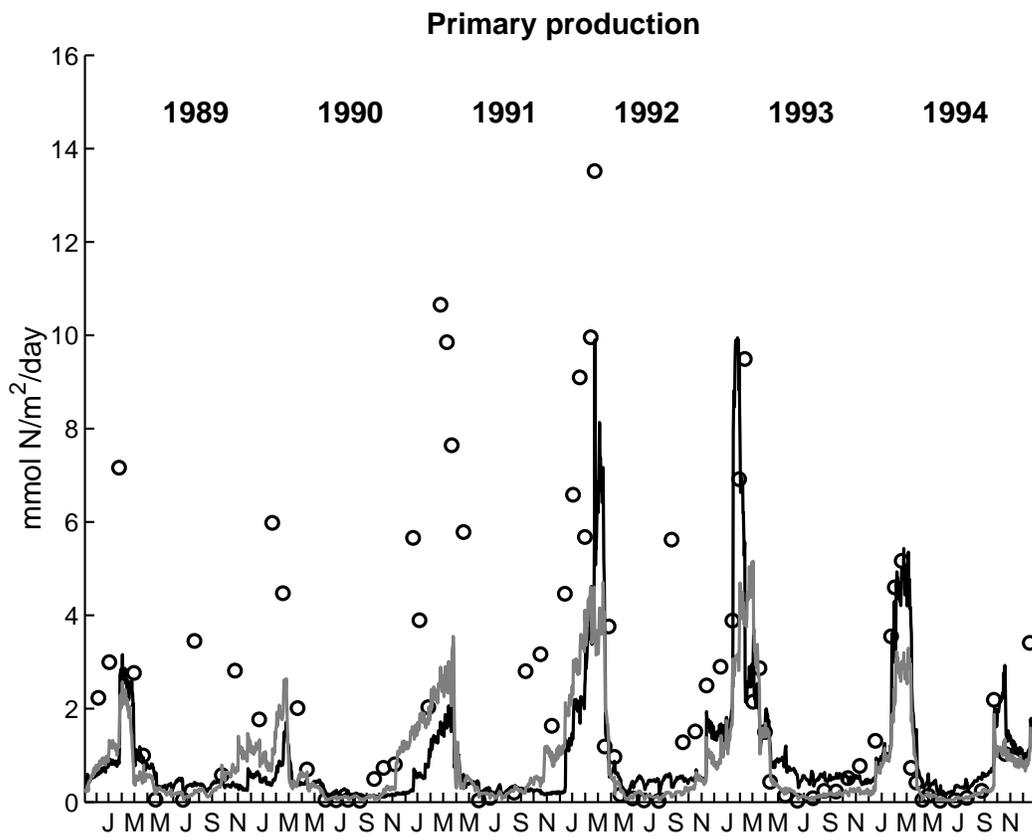


Fig. 7.

Table 1

Adjusted model parameters

| Symbol     | Parameter  | First guess | Unit                |
|------------|--|-------------|---------------------|
| $\mu_1$    | phytoplankton maximum specific mortality rate              | 0.05        | $d^{-1}$            |
| $k_1, k_2$ | half-saturation constants for nutrient and ammonium uptake | 0.5         | $mmol N m^{-3}$     |
| $k_5$      | phytoplankton mortality half-saturation constant           | 0.2         | $mmol N m^{-3}$     |
| $\psi$     | nitrate uptake ammonium inhibition parameter               | 1.5         | $m^3 mmol N^{-1}$   |
| $\alpha$   | initial slope of the $P - I$ curve                         | 0.025       | $m^2 W^{-1} d^{-1}$ |
| $g$        | zooplankton maximum ingestion                              | 1           | $d^{-1}$            |
| $\mu_2$    | zooplankton maximum loss rate                              | 0.3         | $d^{-1}$            |
| $k_3$      | zooplankton ingestion half-saturation constant             | 1           | $mmol N m^{-3}$     |
| $k_6$      | zooplankton loss rate half-saturation constant             | 0.2         | $mmol N m^{-3}$     |
| $\mu_3$    | the bacterial excretion rate                               | 0.05        | $d^{-1}$            |
| $V_b$      | bacterial maximum uptake rate                              | 2           | $d^{-1}$            |
| $k_4$      | bacterial half-saturation const. for uptake                | 0.5         | $mmol N m^{-3}$     |
| $\mu_4$    | detrital breakdown rate                                    | 0.05        | $d^{-1}$            |
| $w$        | detrital sinking rate                                      | 5.000       | $m d^{-1}$          |

Table 2

Fixed model parameters

| Symbol                      | Parameter   | Value | Unit                    |
|-----------------------------|---|-------|-------------------------|
| $k_w$                       | attenuation coefficient of downwelling irradiance | 0.04  | $m^{-1}$                |
| $k_c$                       | light attenuation due to phytoplankton            | 0.03  | $m^2 \text{ mmol}^{-1}$ |
| $\beta_1, \beta_2, \beta_3$ | zooplankton assimilation efficiency               | 0.75  |                         |
| $r_1$                       | zooplankton feeding preferency                    | 0.5   |                         |
| $r_2, r_3$                  | zooplankton feeding preferency                    | 0.25  |                         |
| $\delta$                    | fraction of zooplankton losses going to DON       | 0.2   |                         |
| $\epsilon$                  | fraction of zooplankton losses going to ammonium  | 0.7   |                         |
| $\eta$                      | ammonium:DON uptake ratio                         | 0.6   |                         |
| $R_P$                       | carbon to nitrogen ratio for phytoplankton        | 7     |                         |
| $R_Z$                       | carbon to nitrogen ratio for zooplankton          | 5.5   |                         |
| $R_B$                       | carbon to nitrogen ratio for bacteria             | 5     |                         |

Table 3

Stable estimates for model parameters

| Symbol  | First<br>guess    | Optimized<br>value  | Error<br>variance   | Unit              |
|---------|-------------------|---------------------|---------------------|-------------------|
| $g$     | 1.0               | 0.40                | 0.15                | $d^{-1}$          |
| $\mu_3$ | $5 \cdot 10^{-2}$ | $9 \cdot 10^{-3}$   | $4.5 \cdot 10^{-3}$ | $d^{-1}$          |
| $\mu_4$ | $5 \cdot 10^{-2}$ | $1.1 \cdot 10^{-2}$ | $1.4 \cdot 10^{-3}$ | $d^{-1}$          |
| $\mu_2$ | 0.3               | 0.24                | 0.13                | $d^{-1}$          |
| $k_6$   | 0.2               | 0.20                | 0.08                | $mmol N m^{-3}$   |
| $k_3$   | 1.0               | 2.62                | 1.4                 | $mmol N m^{-3}$   |
| $\psi$  | 1.5               | 0.99                | 0.33                | $m^3 mmol N^{-1}$ |
| $w$     | 5.0               | 4.25                | 2.17                | $m d^{-1}$        |