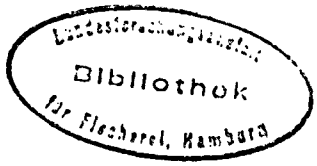

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Theme Session on the North Atlantic Components of Global Programmes: Lessons to ICES-GLOBEC from WOCE/JGOFS(O)

Ecosystem modelling in the North Atlantic JGOFS Programme - what we have learnt

by

M. J. R. Fasham
Southampton Oceanography Centre, Southampton

1. Introduction

The two stated goals of the JGOFS programme can be can be summarised as, firstly, understanding the biological, physical, and chemical processes controlling the carbon cycle within the ocean and, secondly, predicting how this cycle might change under the forcing of global climate change. The JGOFS Science Plan (SCOR, 1990) makes it clear that these goals can only be achieved by means of models. It is impossible to sample the ocean with sufficient temporal and spatial resolution to quantify all the biogeochemical cycles on a global scale and so the observational programme must be focused on providing the necessary information about the key processes involved, so that good mathematical models of these processes can be developed. This is the justification for the rolling programme of world-wide JGOFS process studies and there is no doubt that the JGOFS data sets will, in the coming years, be a fruitful source of information for testing marine biogeochemical models in the same way that the GEOSECS data was for marine chemical models.

In recent years a number of fairly simple ecosystem models have been developed that attempt to model the annual cycle of biological production in the ocean mixed layer (Evans & Parslow 1985; Frost 1987; Fasham et al., 1990; Steele & Henderson 1992). Such models have been used to simulate the seasonal observations from time series stations such as Bermuda Station "S" (Fasham et al., 1990; Steele & Henderson 1993) and Ocean Weather Stations I (Fasham 1993) and P (Frost 1993) with reasonable success. After the initial sense of achievement

has worn off, it has become clear to the modelling community that we now need to take a more objective viewpoint and ask such questions as: "does a model give a good fit to the observations?" and "does model A fit the observations better than model B?". The first of these questions can be approached by first defining a measure of misfit between the model predictions and the observations, and a number of possible measures exist such as least-squares or likelihood functions. Although this a step in the right direction, there is still the problem of deciding whether the value of misfit obtained by a model is good or bad. This is a complex statistical problem that has not yet, to my knowledge, been solved.

Once a model of misfit has been defined then the second question could in principle be answered by comparing the misfit parameters for the two different models. However for this approach to be valid we must have determined the "best' parameter values for each model, a far from simple task. All these models require a fairly large number (10-20) of parameters to specify the ecological processes and estimating values for these parameters is extremely difficult. Some parameters such as phytoplankton and bacterial growth rates or zooplankton grazing and excretion rates can, in principle, be measured at sea by means of suitable experiments. However, even if this is done the modeller requires some annual average of the parameters rather than values for a few times of the year. Some other parameters, such as phytoplankton natural mortality rate or detrital remineralisation are, at present, almost impossible to measure accurately. The approach of most modellers to this problem has been to use experimentally-determined parameter values where these are available and then adjust some or all of the remaining parameters until the model shows a good agreement with the observation set. There are two problems with this approach. The first is that, with a large parameter set, it is often difficult to get the model to give a good fit to all the observation set with such a hit-and-miss method. When this happens one is uncertain if this is due to inadequacies in the model or whether the correct part of the parameter space has been missed. What is obviously needed is a more rational and automated approach and a number of techniques are now available such as simulated annealing (Hurtt & Armstrong, 1996) and nonlinear optimisation (Fasham & Evans, 1995). This paper will describe some results using the latter technique to compare the fit of different models to a given data set and the fit of a single model to a number of different data sets.

2. Methods

It is first necessary to define the measure of misfit. Fasham & Evans (1995) chose a function that minimised the sum of squared deviations between model

predictions and observed values. We further assumed that the variance increases as the square root of the actual value and so the misfit measure *Tobs* was defined as

$$Tobs = \Sigma \Sigma \; w_{ij}.(\sqrt{Xobs_{ij}} - \sqrt{Xmod_{ij}})^2$$

where $Xobs_{ij}$ and $Xmod_{ij}$ are the observed and simulated values respectively of a state variable i at time t_j w_{ij}. is a weight, and the double summation is over all the state variables and all observation times. As we will be comparing the fit of models to observation sets with varying numbers of observations it is useful to calculate an average misfit per degrees of freedom, *Tavg = Tobs/(nobs -npar)* where *nobs* is the number of observations and *npar* the number of model parameters.

We also have prior ideas about what the parameter values should be: both intrinsic bounds on parameters (fractions lie between 0 and 1; grazing rates are not negative) and a target value that we would choose in the absence of data, but ignore if the data strongly suggest another value. These ideas are incorporated in a penalty function depending on three terms: T, the suggested or target value of the parameter, and U and L, its upper and lower bounds. If p is a trial parameter value with estimated variance v, then a term

$$P(p) = \frac{T-p}{(p-L)\,v} \qquad L < p \leq T$$

$$= \frac{p-T}{(U-p)\,v} \qquad T \leq p < U$$

is added to *Tobs* to give a combined penalty function for the minimisation algorithm. If the variance v is large (a value of 10 was used), then the penalty is small except very near the bounds where it grows without bound. This would ensure that the majority of the misfit came from observation misfit rather than parameter misfit.

Once we have chosen a function to minimise, wandering through parameter space in search of a minimum is a fairly standard, if lengthy, operation. The only small complication is that we do not use methods that rely on gradients of the function. This is because we have found numerical differentiation of numerical solutions of systems of differential equations, where automatic step size control changes the points at which the solution is evaluated, to be unreliable. We therefore used Powell's conjugate direction method, more or less as implemented by Press et al. (1992).

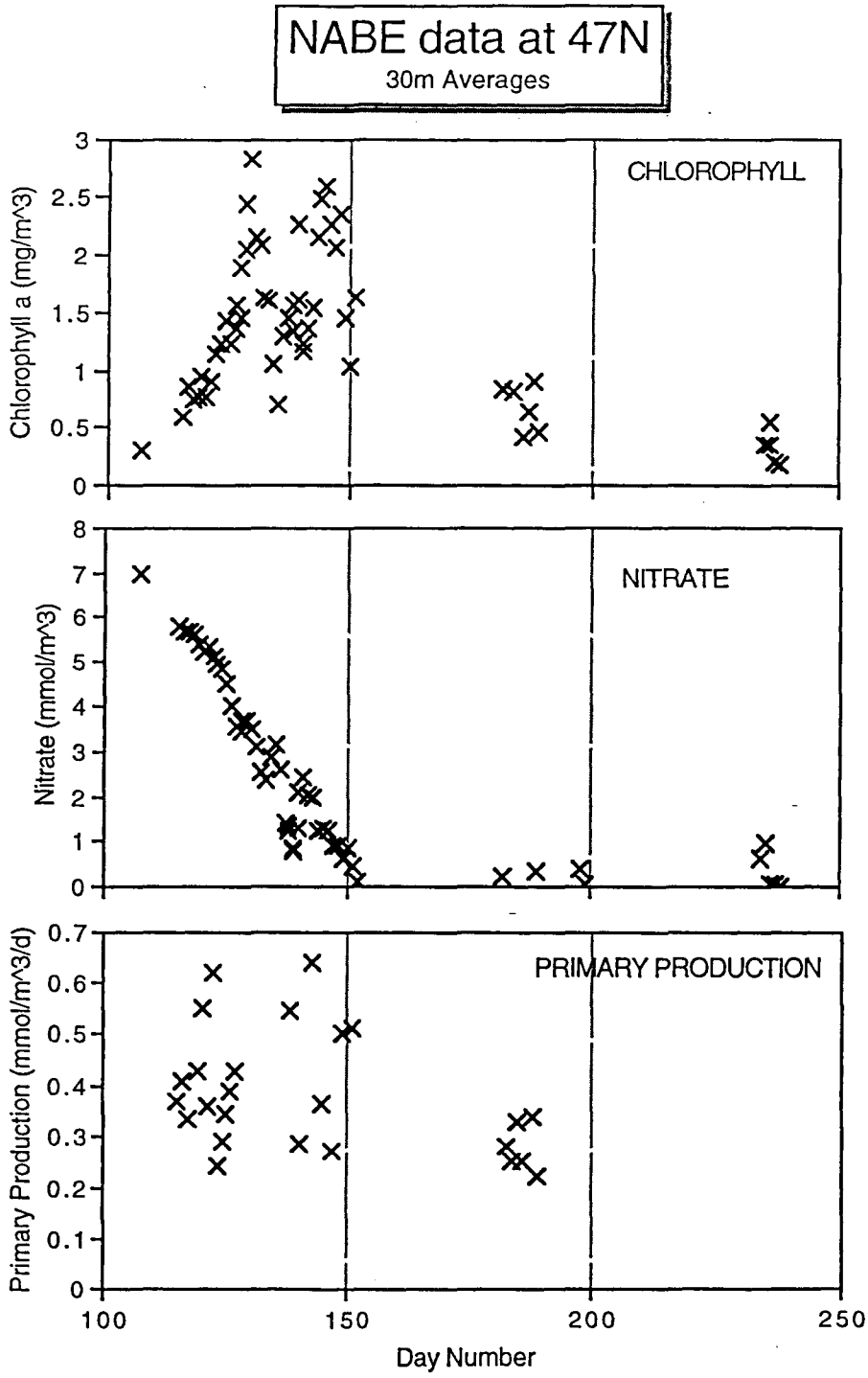


Fig. 1. Observations of from top to bottom of (a) phytoplankton biomass , (b) nitrate concentration , and (c) primary production obtained at 47° 20°W during the JGOFS North Atlantic Bloom Experiment.

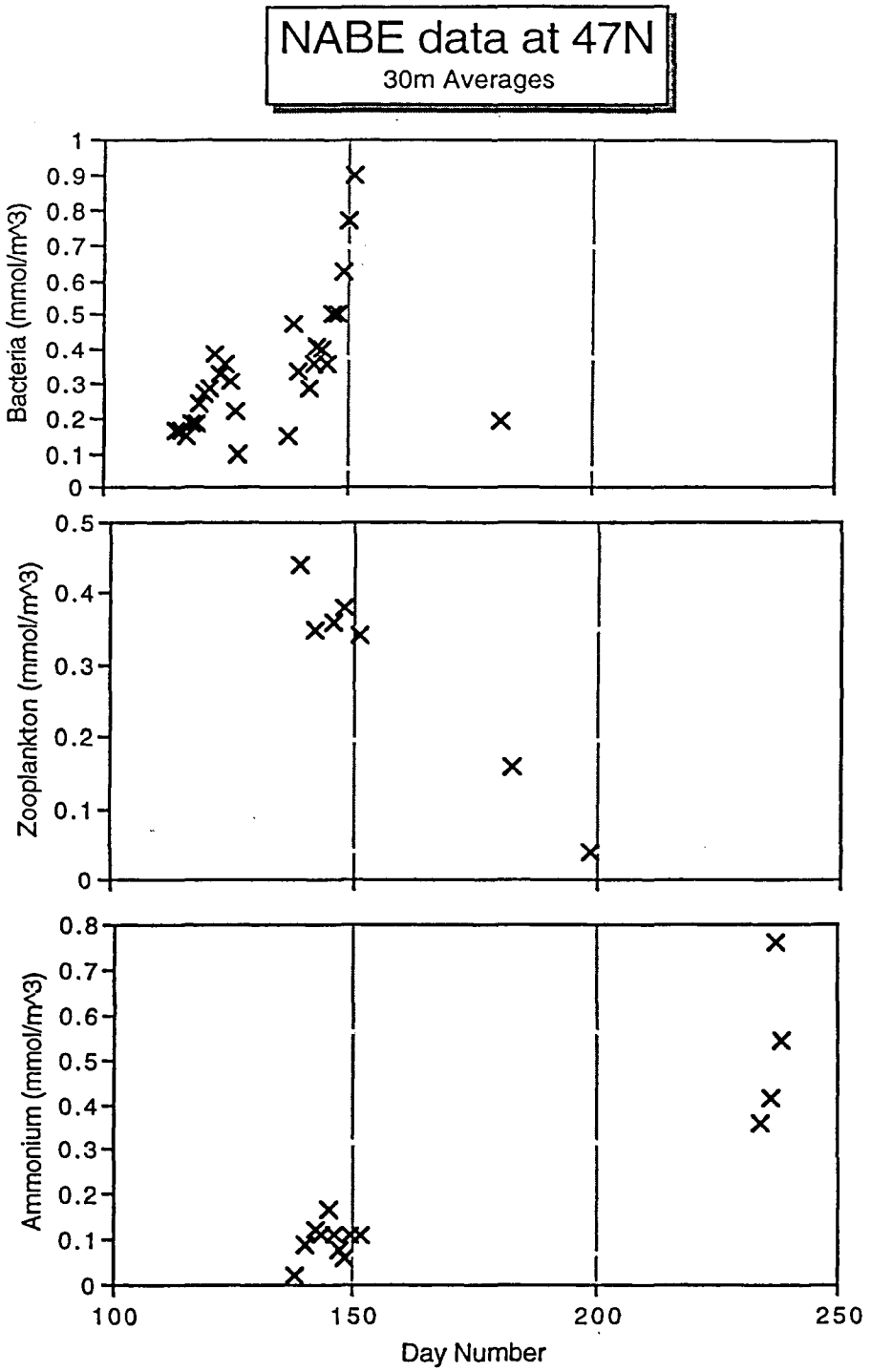


Fig. 1 (contd.). Observations of from top to bottom (d) bacterial biomass, (e) zooplankton biomass, and (f) ammonium concentrations.

3. The observation set

The techniques were tested with an observation set derived from measurements made during the 1989 JGOFS North Atlantic Bloom Experiment at 47° 20°W (Ducklow & Harris 1993; Lochte et al. 1993). The bulk of the data covered the period from 24th April-31st May obtained on two US cruises on

Atlantis *II* and one German cruise on *Meteor* . The *Meteor* cruise covered the period during which *Atlantis II* was in port, ensuring a complete coverage of the spring bloom period. Some summer data were also obtained from British and Dutch cruises. To provide data for comparison with the model, averaged values within the top 30m were calculated. Standard conversion factors were used to convert observations to nitrogen units (Fasham & Evans, 1995). Good time series for phytoplankton chlorophyll, nitrate, and bacteria (figs. 1a,b, & d) were available but the data sets for primary production, ammonium and zooplankton were more limited (figs. 1c,e, & f).

A more detailed plot of the spring bloom period shows that the spring bloom is made up of two separate peaks (fig. 2). As the *Meteor* and *Atlantis* were not occupying exactly the same position during their sampling, this double peak might have been caused by spatial variability. However, the nitrate data show a good continuity between all three cruises and also the silicate was almost totally utilised during the period of the first peak. This strongly suggests that the first bloom was due to diatoms and this is supported by phytoplankton species counts made on the Meteor cruise (Lochte et al. 1993).

4. The Ecosystem models

The three ecosystem models that were used for the optimisation experiments are all based on the mixed layer nitrogen model of Fasham, Ducklow & McKelvie (1990; hereinafter referred to as FDM). The equations governing the FDM model are given in the original paper and only a brief summary of the model structure will be given here.

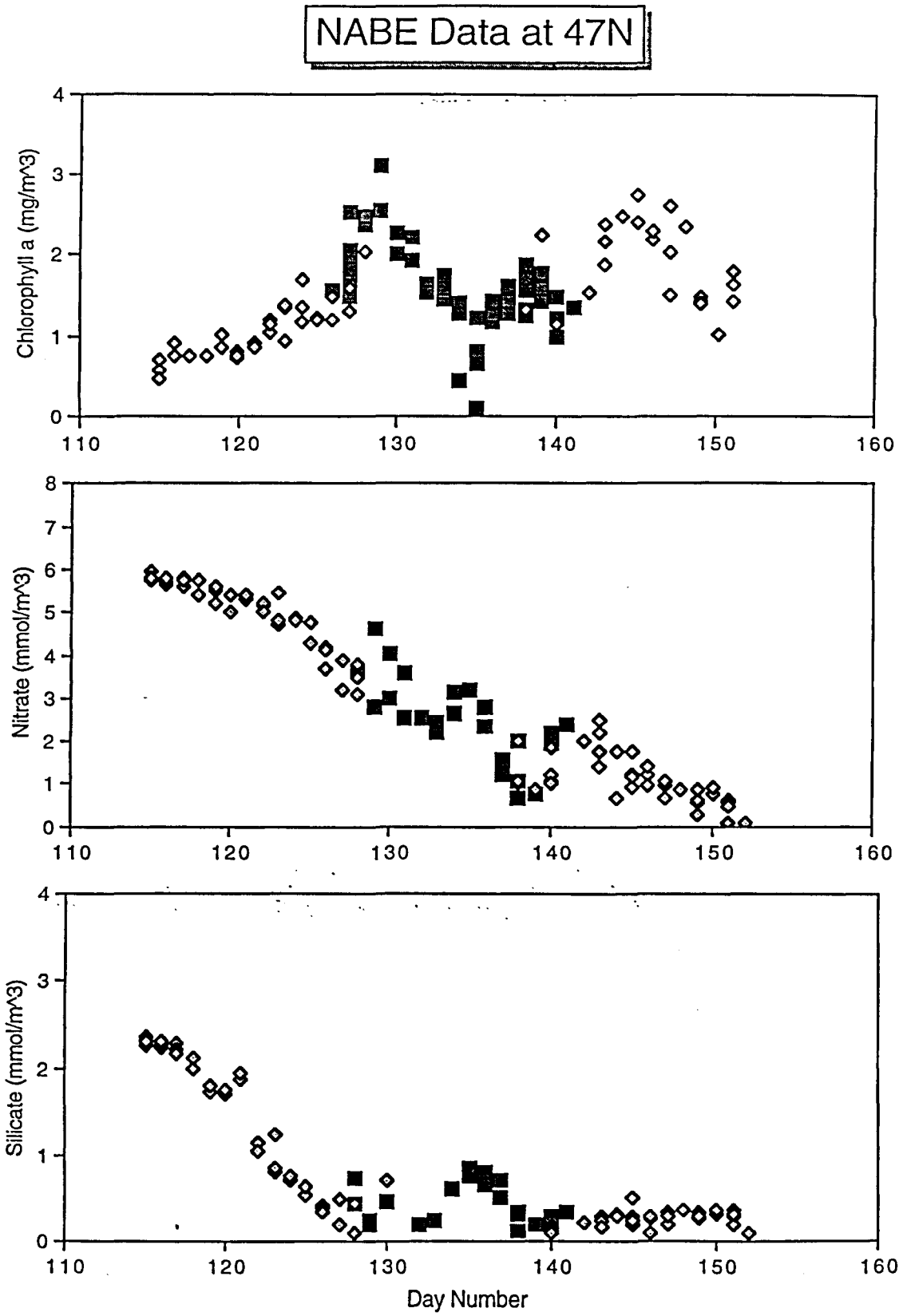


Fig. 2 Detailed time series of phytoplankton chlorophyll, nitrate, and silicate concentrations obtained at 47° 20°W during the JGOFS North Atlantic Bloom Experiment. Meteor observations are squares and Atlantis II observations diamonds.

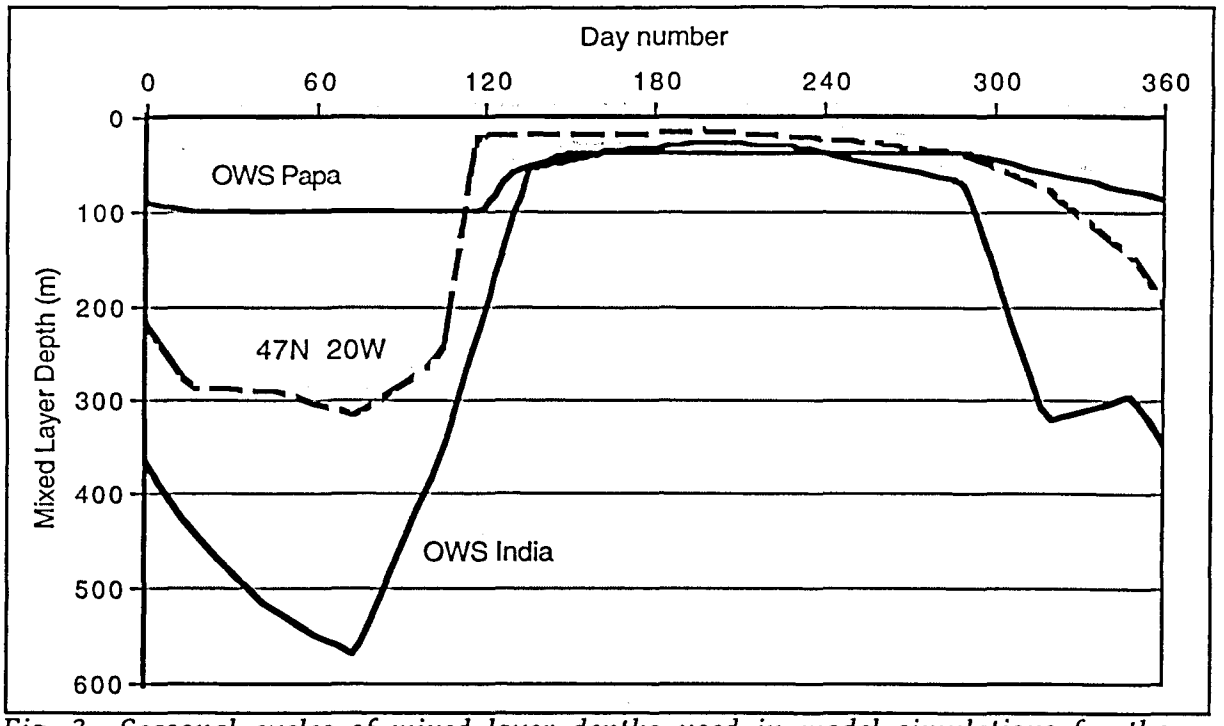


Fig. 3 Seasonal cycles of mixed layer depths used in model simulations for the NABE site at 47°N 20°W, OWS Papa and OWS India.

The seasonal changes in mixed layer depth are not explicitly modelled but are assumed to be known from observations. For modelling the seasonal cycle at 47°N 20°W climatic mixed layer depths (Levitus 1982) were supplemented by ship's observation for the period of the spring thermocline development (fig. 3). The deepening of the mixed layer throughout the late autumn and winter entrains nitrate from below the mixed layer that fuels the new primary production. The amount of nitrate entrained, and therefore the nitrate concentration at the start of the spring bloom, depends on the assumed vertical nitrate gradient below the mixed layer (this is specified by the equation $N = a + bz$, where z is depth and a,b are parameters of the model) . Mixing of entities across the pycnocline can also be effected by various processes and these processes are all parameterised by a constant mixing rate. The other physical forcing function is the solar radiation which is parameterised by the standard astronomical formulae (Brock 1981) and a model for the atmospheric transmittance of the cloud (Evans & Parslow 1985) with a constant fractional cloudiness. Light transmittance through the water column was parameterised by Beer's law with a water attenuation coefficient and phytoplankton self-shading coefficient. All the parameters describing these processes were estimated by the optimisations apart from the mixed layer depths.

The three ecosystem models used were:

Model 1 (fig. 4a)

This is a simplification of the original FDM model obtained by excluding bacteria and labile DON. It was assumed that detrital breakdown within the mixed layer was recycled directly to ammonium rather than via DON and bacteria. The number of model parameters to be estimated by the optimisation was 21.

Model 2 (fig. 4b)

This is the standard FDM model with the one alteration that zooplankton mortality is parameterised by a quadratic function of zooplankton biomass rather than a linear function (see below for details). Number of model parameters = 28.

Model 3 (fig. 4c)

In this model the phytoplankton have been split into diatoms and other non-diatom phytoplankton. The growth of diatoms is assumed to be jointly limited by nitrogen and silicate. Silicate uptake by diatoms was assumed to be a constant multiple of the total nitrogen uptake (ammonium plus nitrate). Number of model parameters = 39.

The functional relationship between phytoplankton growth rate and light and the interaction between ammonium and nitrate uptake was described in FDM. All models have only one zooplankton compartment that feeds on phytoplankton, bacteria, and detritus (and in the case of model 3, two types of phytoplankton). The feeding preferences for the various prey change dynamically as a function of the relative proportion of the prey and this parameterisation acts as a stabilising property of the model equations (FDM). Losses due to faecal pellet egestion were parameterised by an assimilation efficiency, while excretion was assumed to be a linear function of biomass.

The parameterisation of the zooplankton mortality is not trivial as it represents the effect of un-modelled higher predators and is a closure term for the ecosystem model. Steele & Henderson (1992) have shown that the mathematical form of this closure term can have a large influence on the dynamics of a model and they favoured a mortality function that was a quadratic function of zooplankton biomass. Recently, Fasham (1995) has provided further support for the quadratic model and it was used in all three models; this is the one difference between model 2 the FDM model. A fraction of the zooplankton mortality flux is exported as fast-sinking detritus from the mixed layer while the remainder is recycled to ammonium within the mixed layer.

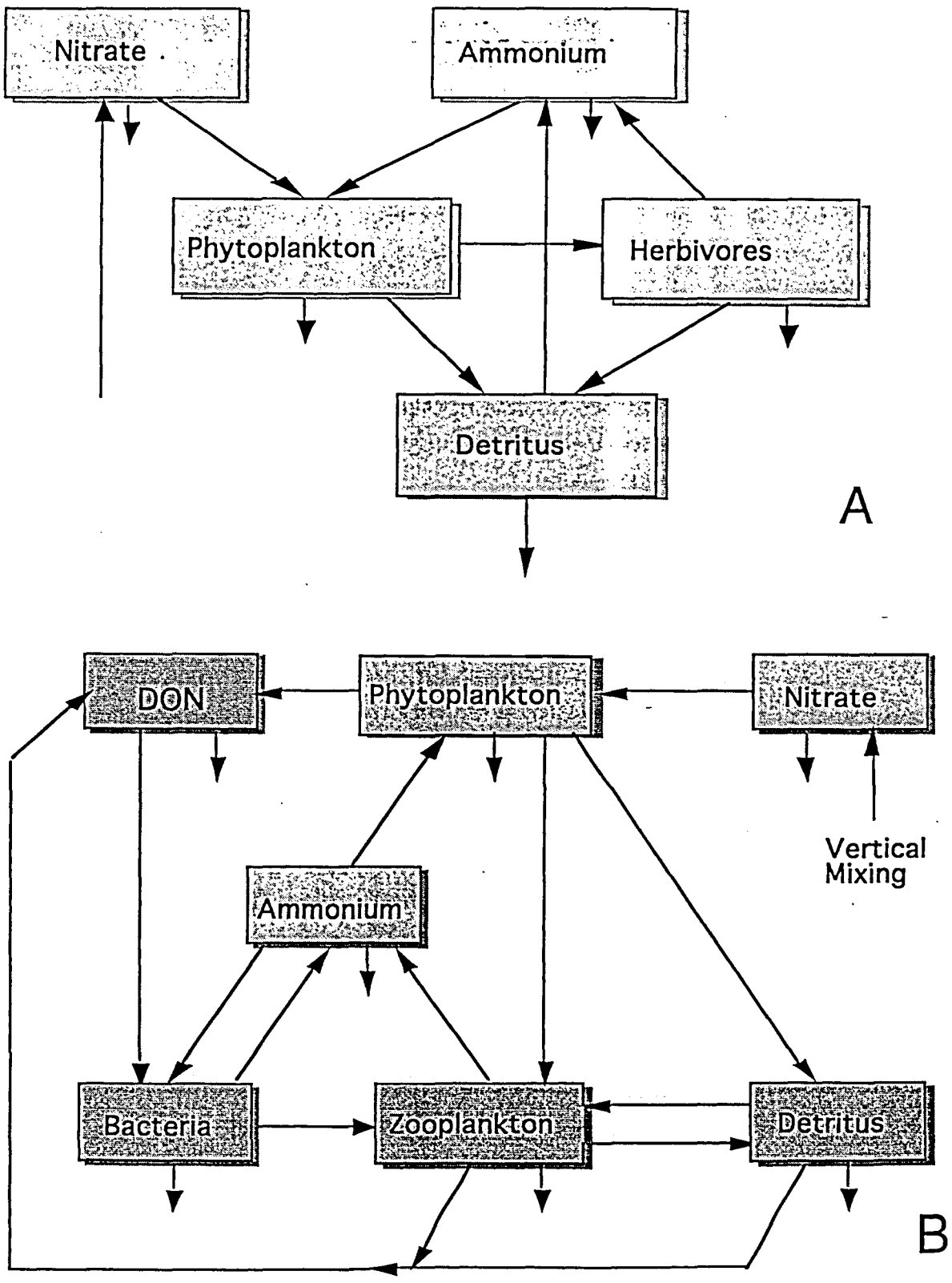
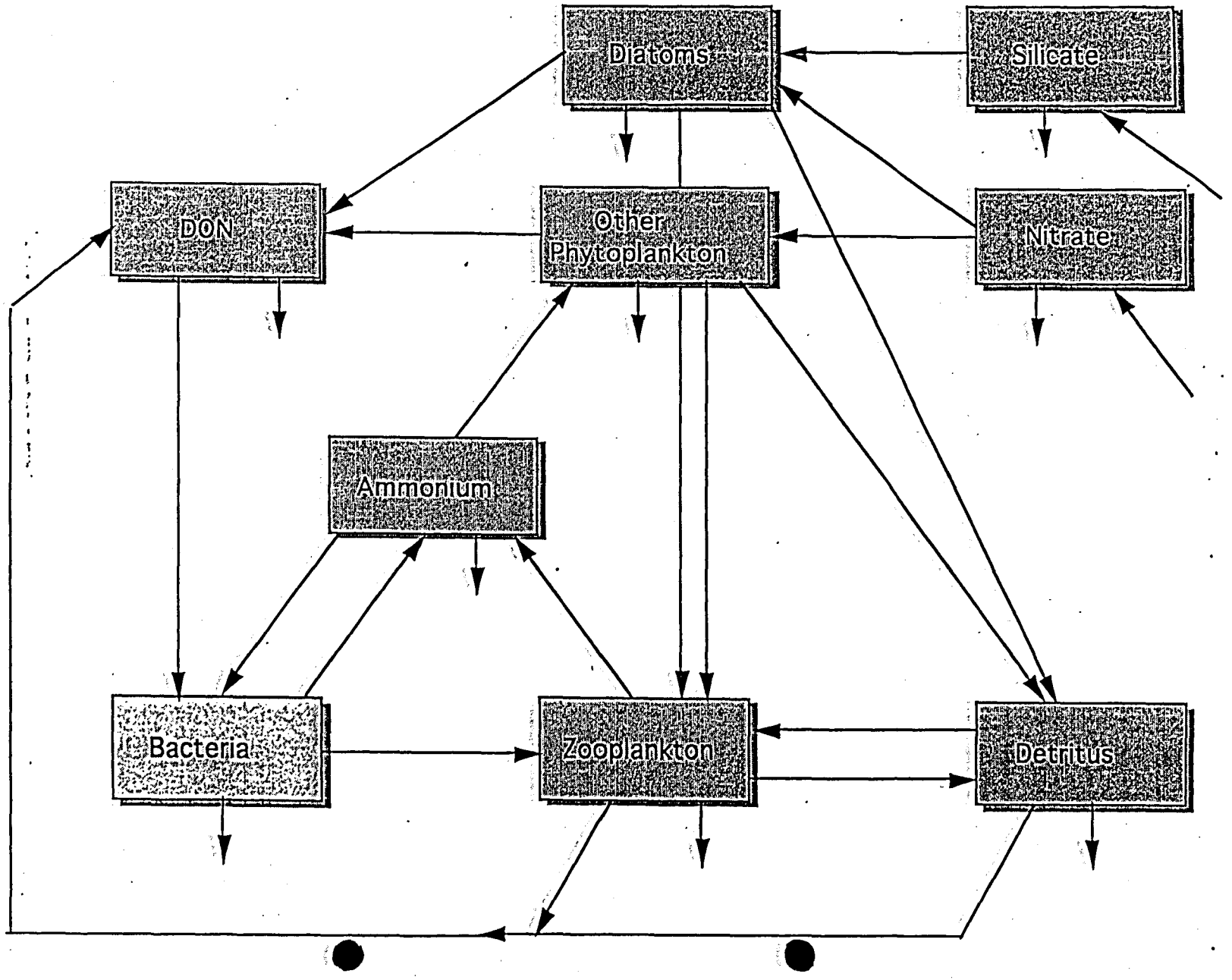


Fig. 4 Flow diagrams for A) five-compartment models and B) seven-compartment FDM model


Diatoms
Silicate
DON
Other Phytoplankton
Nitrate
Ammonium
Bacteria
Zooplankton
Detritus

The bacteria (models 2 & 3 only) are modelled as in FDM.

Model detritus is derived from faecal pellets and dead phytoplankton and a fraction of this material sinks out of the mixed layer to the ocean interior. However, detritus can also be recycled within the mixed layer by two mechanisms, namely its reingestion by zooplankton or its breakdown into DOM and subsequent uptake by bacteria. In the models the fate of the detritus is determined by two parameters, the detrital sinking rate and the breakdown rate of detritus to ammonium (model 1) or DON (models 2 & 3).

The model equations were solved with a variable time-step algorithm and were run for 2 years to achieve a repeating annual cycle. The results from the third year of the simulation were used to calculate the misfit from the observations.

5. Fit of models to the observation set

a) Model 1: basic five compartment model

The optimal fit of model 1 to the phytoplankton, zooplankton, nitrate, ammonium, and primary production observations (*nobs*=150) yielded *Tobs* and *Tavg* of 6.2 and 0.05 respectively. The model predicted the nitrate observations very successfully (fig. 5); this is not too surprising given that the spring nitrate decline was so well covered by the observations and that the nitrate values have the highest magnitude range and so the greatest reduction in the misfit can be achieved by fitting these observations closely. It was found that the optimisation method nearly always gave excellent fits to the nitrate observations and this is very useful as it ensures that there is a good temporal match between model and observations for the main factor controlling the spring bloom. The initial spring increase in phytoplankton was also modelled well but the double peak structure was not (fig. 5). This is hardly surprising bearing in mind that the model has only one class of phytoplankton so that the optimisation averaged through the two blooms and yielded a model peak that coincided with the minimum between the two observed chlorophyll peaks.

The predicted primary production values were within the range of observations during the spring bloom, although they were still less than the observed values in July. Martin *et al.* (1993) demonstrated that a large amount of the day-to-day variability in primary production was due to daily variations in

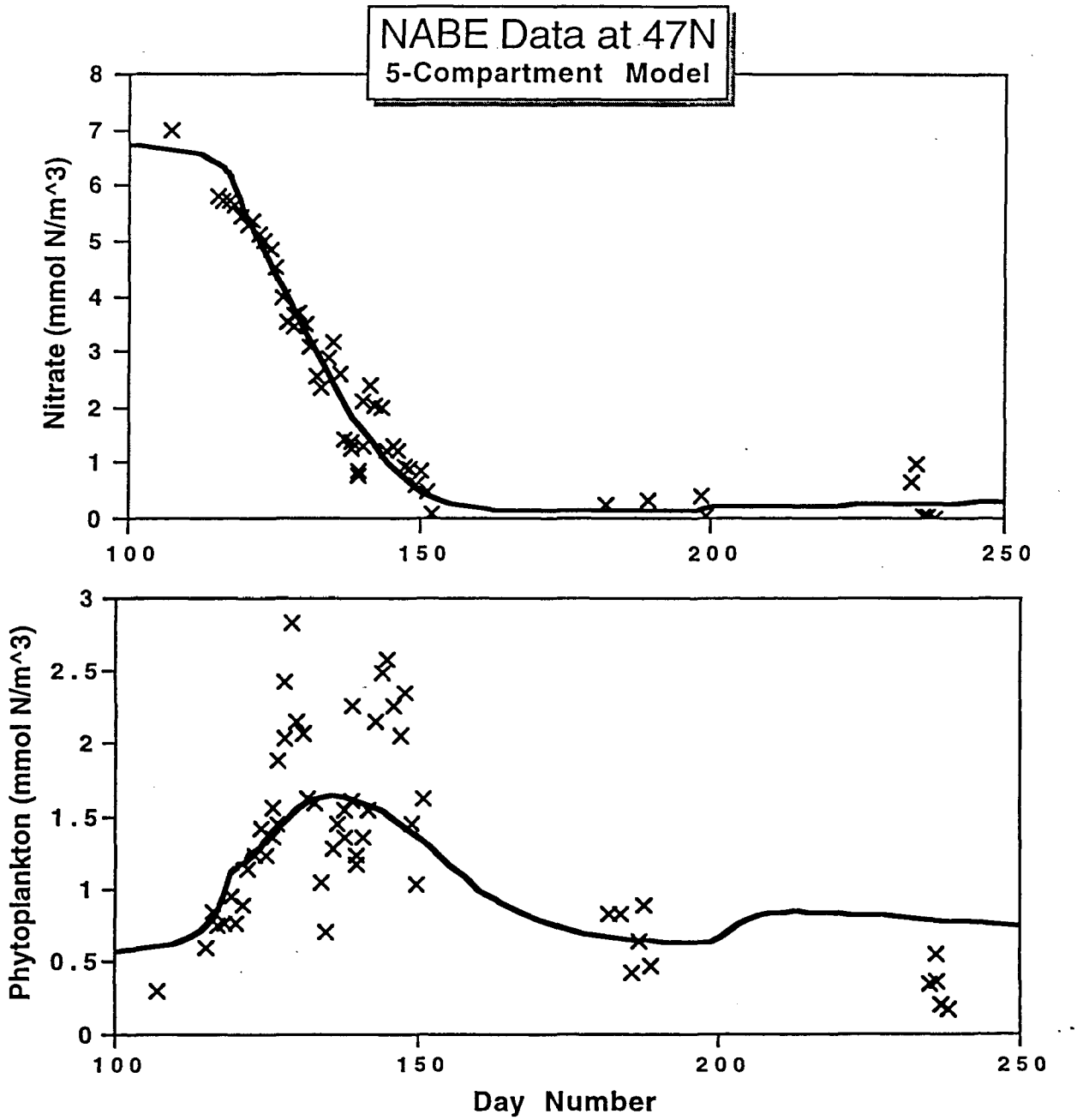


Fig. 5. Fit of the 5-compartment model to observations of phytoplankton biomass (bottom) and nitrate concentration (top) at the NABE site at 47°N 20°W.

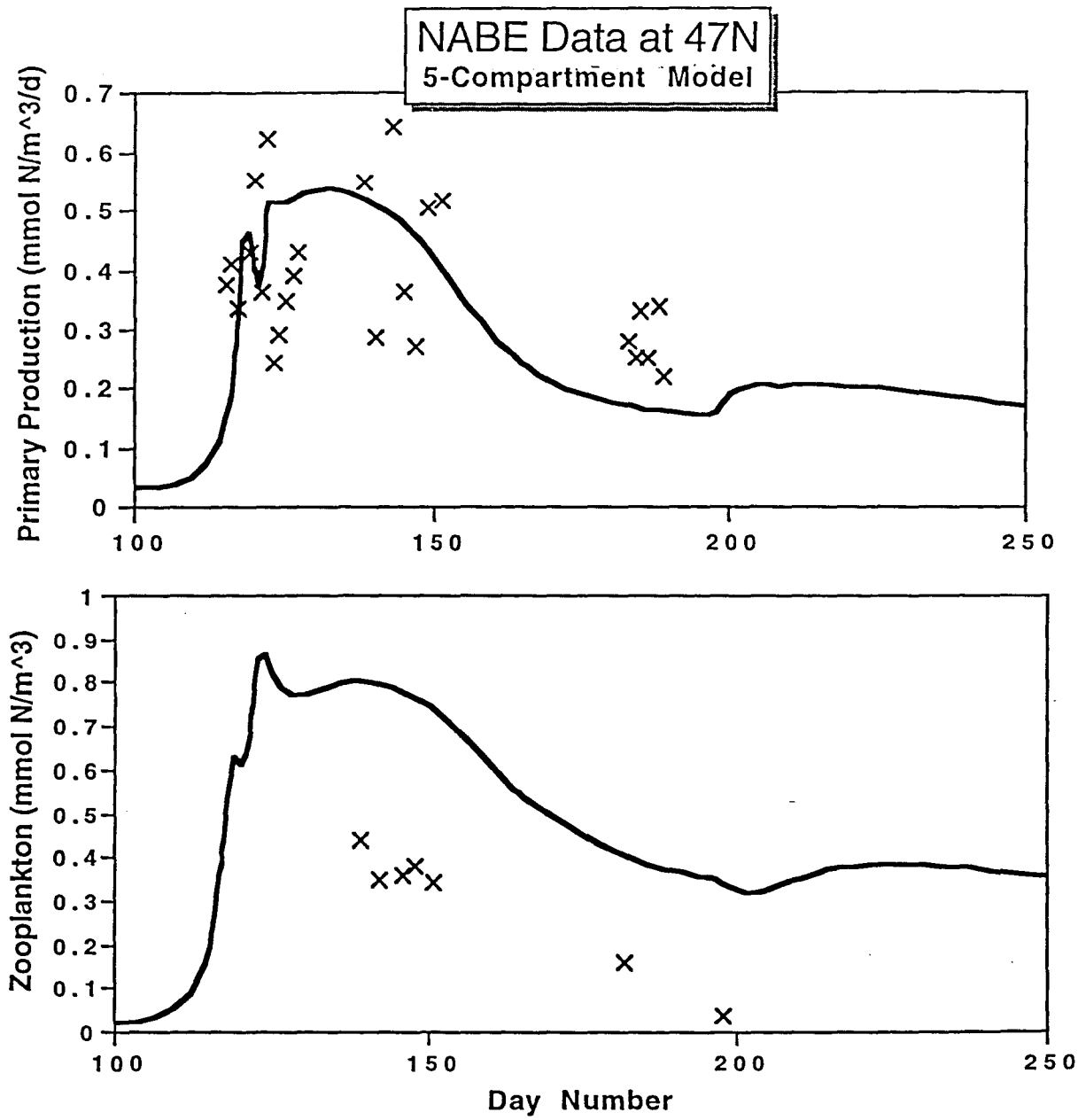


Fig. 5 (contd.). Fit of 5-compartment model to zooplankton (bottom) and primary production (top) observations.

cloud cover that could not be reproduced by the model which assumed a constant cloudiness.

A failing of the model (and models 2 & 3) was that it predicted zooplankton biomass that was more than twice the observed values. Fasham & Evans (1995) showed that it was possible to get a better fit to the limited number of zooplankton observations by assigning them a weight of ten times the other observations. However, this resulted in primary production being greatly underestimated. The reason for this is that the lower zooplankton biomass

causes zooplankton excretion and thereby regenerated production to be much lower. This is obviously a problem that requires further study and it is not at present clear whether this discrepancy is due to inadequacies in the models or to an underestimation of microzooplankton biomass by the present observations. For example, it appears that the biomass of some groups of microzooplankton (e.g. copepod nauplii) may not have been included in some of the published microzooplankton biomass estimates (Harris, pers. comm.).

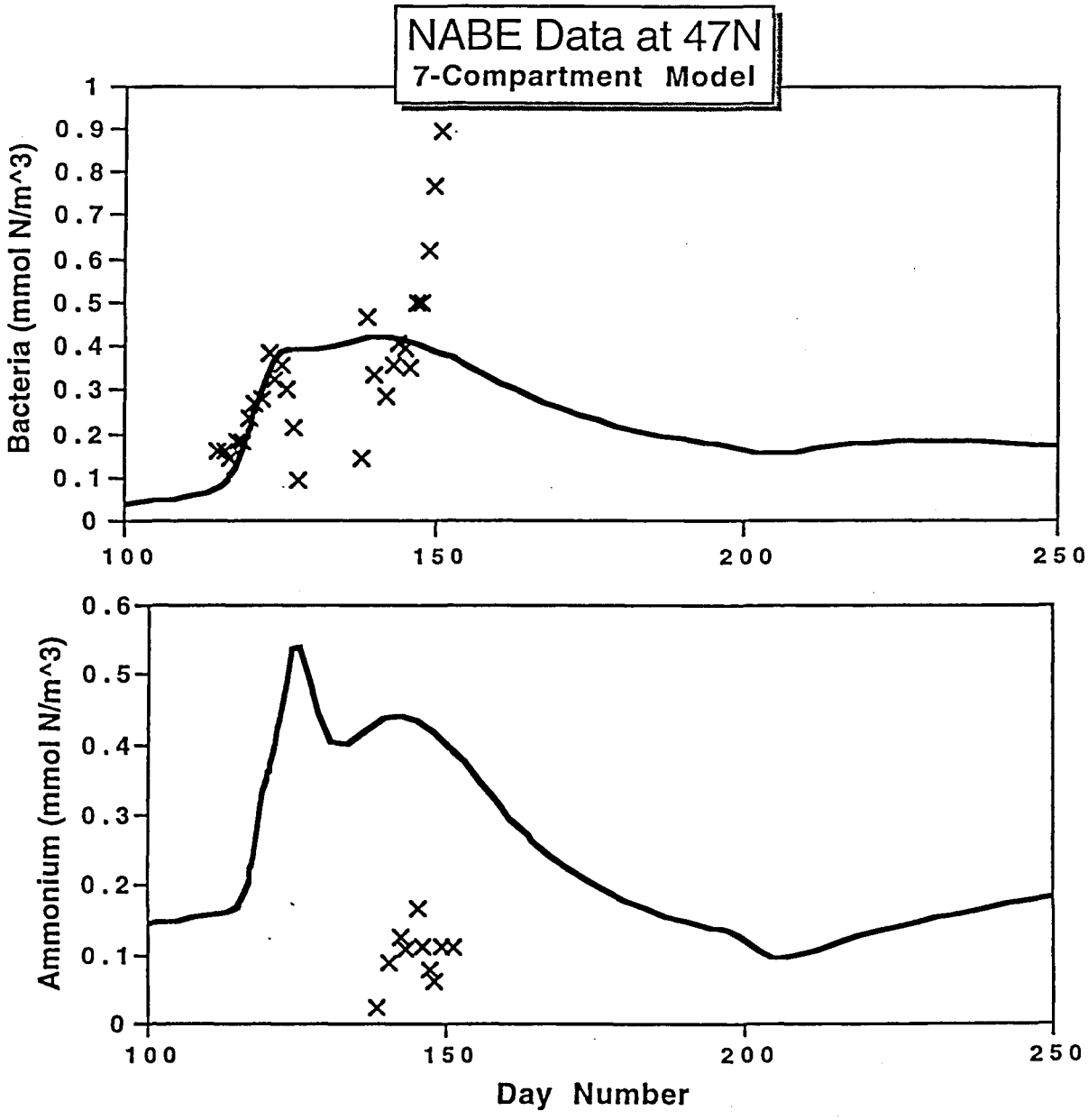


Fig. 6 Fit of the 7-compartment model to bacteria biomass (top) and ammonium (bottom) observations from the NABE site at 47°N 20°W.

b) Model 2: including bacteria

Model 2 was optimised to the observations set used for model 1 with in addition the observations of bacterial abundance obtained on the two *Atlantis II* cruises (*nobs*=178). The values of *Tobs* and *Tavg* were 7.84 and 0.05 respectively. Note that the overall fit of the model as represented by the parameter *Tavg* was no better than for the 5-compartment model. The fit to the nitrate, phytoplankton and primary production observations was almost identical to that of model 1, while the model 2 zooplankton values were slightly higher than those of model 1. It appears therefore that adding bacteria to our model has not improved our ability to model these variables. The fit of the model to the bacteria data was good for the initial bacterial bloom but poor for the remaining period for which observations were available (fig. 6a). The model over-estimated ammonium concentrations (fig. 6b) as, in fact, did all three models.

c) Model 3: diatoms and silicate

In order to be able to use model 3 it was necessary to partition the phytoplankton chlorophyll observations between diatoms and other phytoplankton. This was done by calculating a linear regression of the fraction of phytoplankton biomass attributed to diatoms against time using the observations made by Decker (see Lochte *et al.* 1993) on the *Meteor* cruise and suitable extrapolations for the two *Atlantis II* cruises. The observation set now contained 263 observations and the resulting optimisation gave *Tobs* and *Tavg* values of 15.1 and 0.06 respectively.

The average fit of the model 3 was actually slightly worse then either of the previous models although there are some aspects of the fit that were distinct improvements. The addition of two phytoplankton compartments made a significant change to the simulation of total phytoplankton (diatoms plus other phytoplankton) for the spring bloom period (fig. 7a). The modelled phytoplankton now showed two peaks at the approximately the same times as the observed peaks in phytoplankton chlorophyll, although the model underestimated both the peak magnitudes and overestimated the minimum value between the two peaks. The first of these peaks was due to diatoms (fig. 7b) and the model also gave an excellent fit to the silicate observations (fig. 7c). The modelled bacteria also showed two peaks giving a better overall fit to the bacteria observations than models 1 or 2 (fig. 7d).

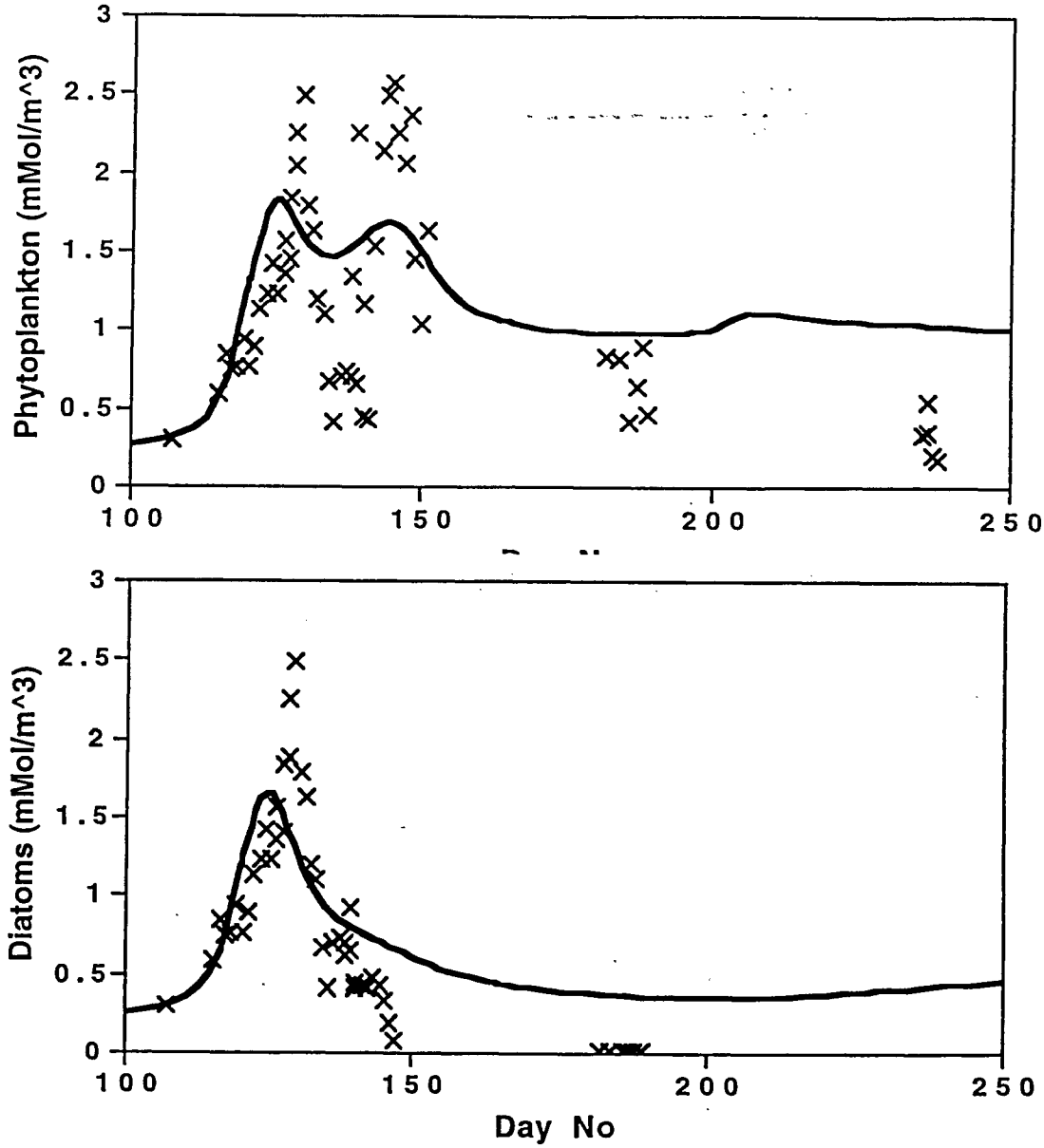


Fig 7. Fit of the 9-compartment diatom model to observations of (a) total phytoplankton biomass (top) derived from chlorophyll measurements, and (b) diatom biomass (bottom) derived from measurements of fractional diatom abundance.

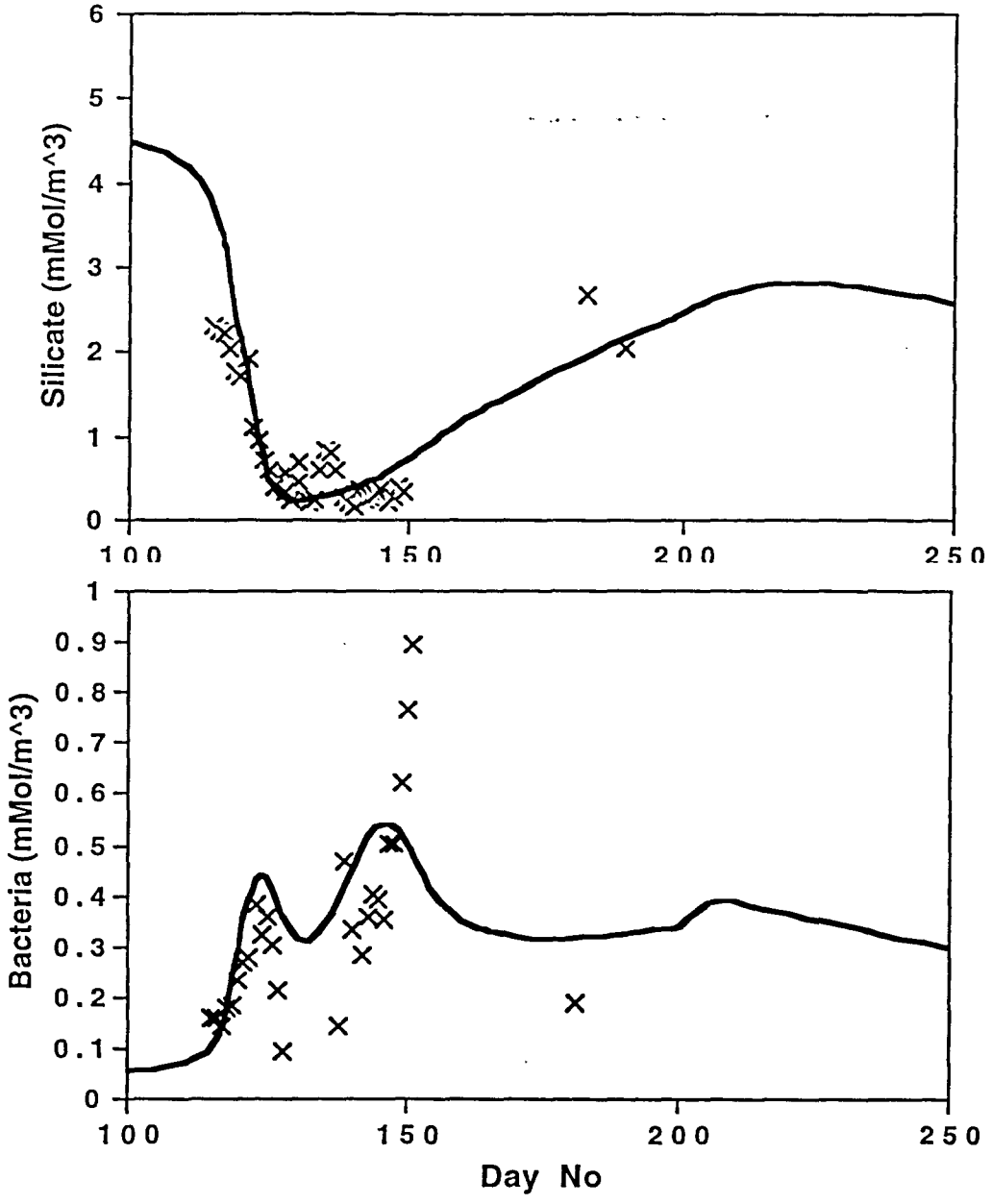


Fig. 7 (contd.). Fit of the diatom model to observations of (c) silicate concentration (top) and (d) bacterial biomass (bottom) obtained at the NABE site at 47°N 20°W.

6. Fit of 5-compartment model to other data sets

One of the criteria for a successful model that has been proposed is whether it is capable of fitting time series observations from different areas of the world ocean. The issue here is whether the differences in the seasonal cycles of primary and secondary production are mainly determined by physical forcing and so can be represented by a relatively simple ecosystem model, or whether significant differences in the species and community structure would rule this out. An obvious test for a such a geographically robust model would be whether

it can reproduce the very different seasonal cycles observed in the subarctic North Atlantic and North Pacific. This was tested by fitting the 5 compartment model (model 1) to observations from Ocean Weather Station (OWS) Papa in the North Pacific and OWS India in the North Atlantic.

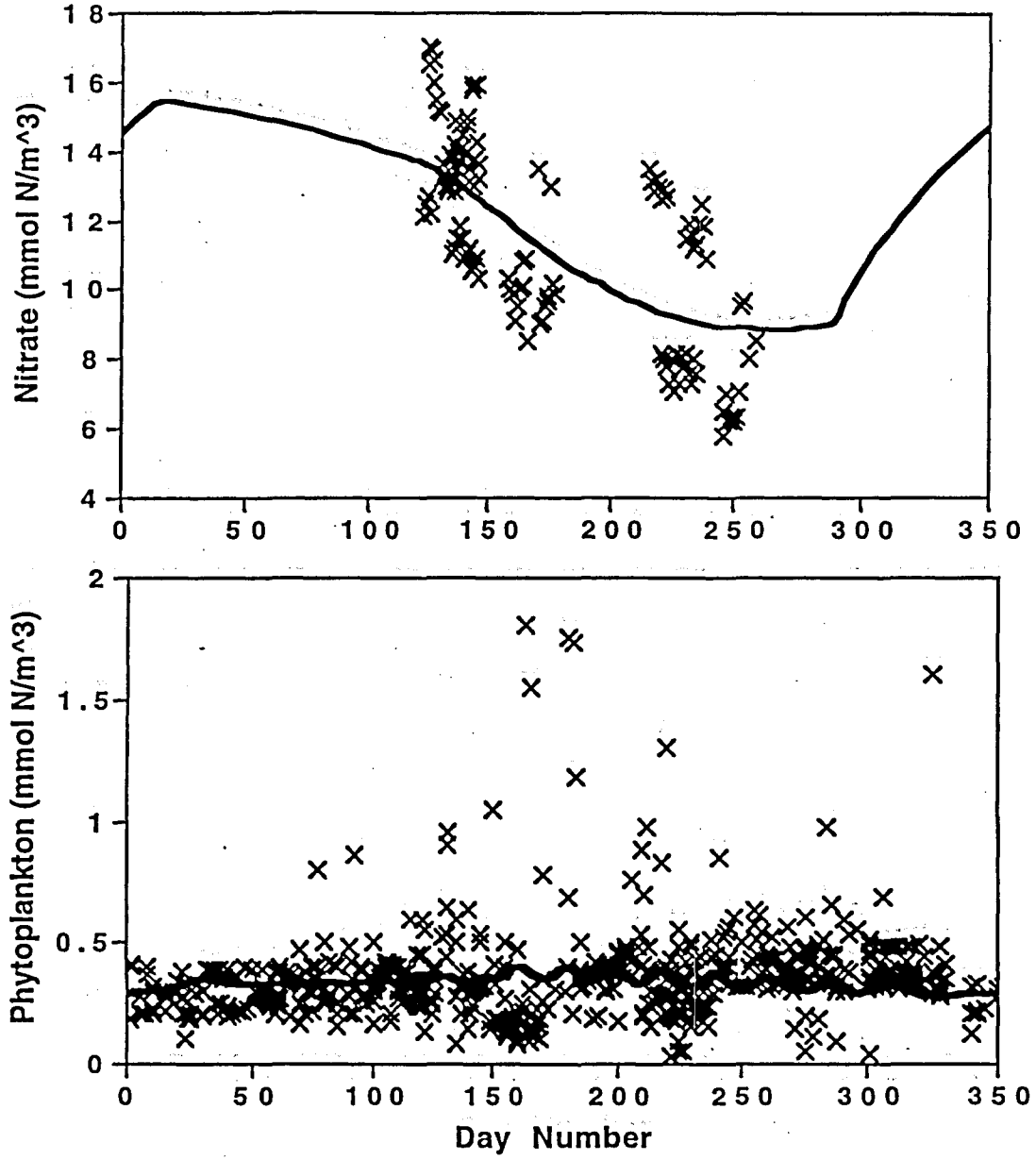


Fig. 8. Fit of 5-compartment model to observations of phytoplankton biomass (bottom) and nitrate (top) concentrations at OWS Papa.

The observations from OWS Papa used in this test consisted of a number of years of phytoplankton observations plus three years of nitrate observations (*nobs*=231) obtained on the SUPER cruises (Miller, 1993). The optimum fit of the model gave values of *Tobs* and *Tavg* of 22.69 and 0.10 respectively. The results (fig. 8) show that the simple five-compartment model was quite capable of

reproducing the almost invariant chlorophyll levels and the high summer nitrate values that typify the subarctic Pacific seasonal cycle. It was very interesting that the optimisation produced a value for the photosynthetic efficiency (initial slope of the P-I curve) that was higher than those obtained for either the 47°N NABE site or OWS India. This is in agreement with other attempts to model the OWS Papa cycle (Fasham, 1995; Frost, 1993).

Fasham (1993) used a modified FDM model to simulate with some success the observations made at OWS India during 1972 (*nobs*=189). The parameter set used was based mainly on the values used to model the annual cycle at Bermuda, although a density dependent phytoplankton and zooplankton mortality was introduced to cope with the very low winter primary production caused by the deep winter mixed layer depths. An interesting feature of the model results was a limit cycle behaviour during the summer when the mixed layer was shallow. The chlorophyll values also showed a number of bloom peaks during the summer, although this may have been due to species succession rather than classical limit cycle dynamics. The phytoplankton, nitrate observations , and primary production were used for the optimisation giving *Tobs* and *Tavg* values of 55.7 and 0.29 respectively.

The most intriguing aspect of the model simulations is that the 5-compartment model also produced a limit cycle (fig. 9) showing that the previous result of Fasham (1993) was not model-dependent. This conclusion also raises the interesting point as to why, bearing in mind the double phytoplankton peak at the 47°N site, a limit cycle solution could not be obtained for that data set. Some recent theoretical work (Ryabchenko et al., in press) suggests that this may be due to the large sub-surface nitrate gradients at OWS India compared to 47°N.

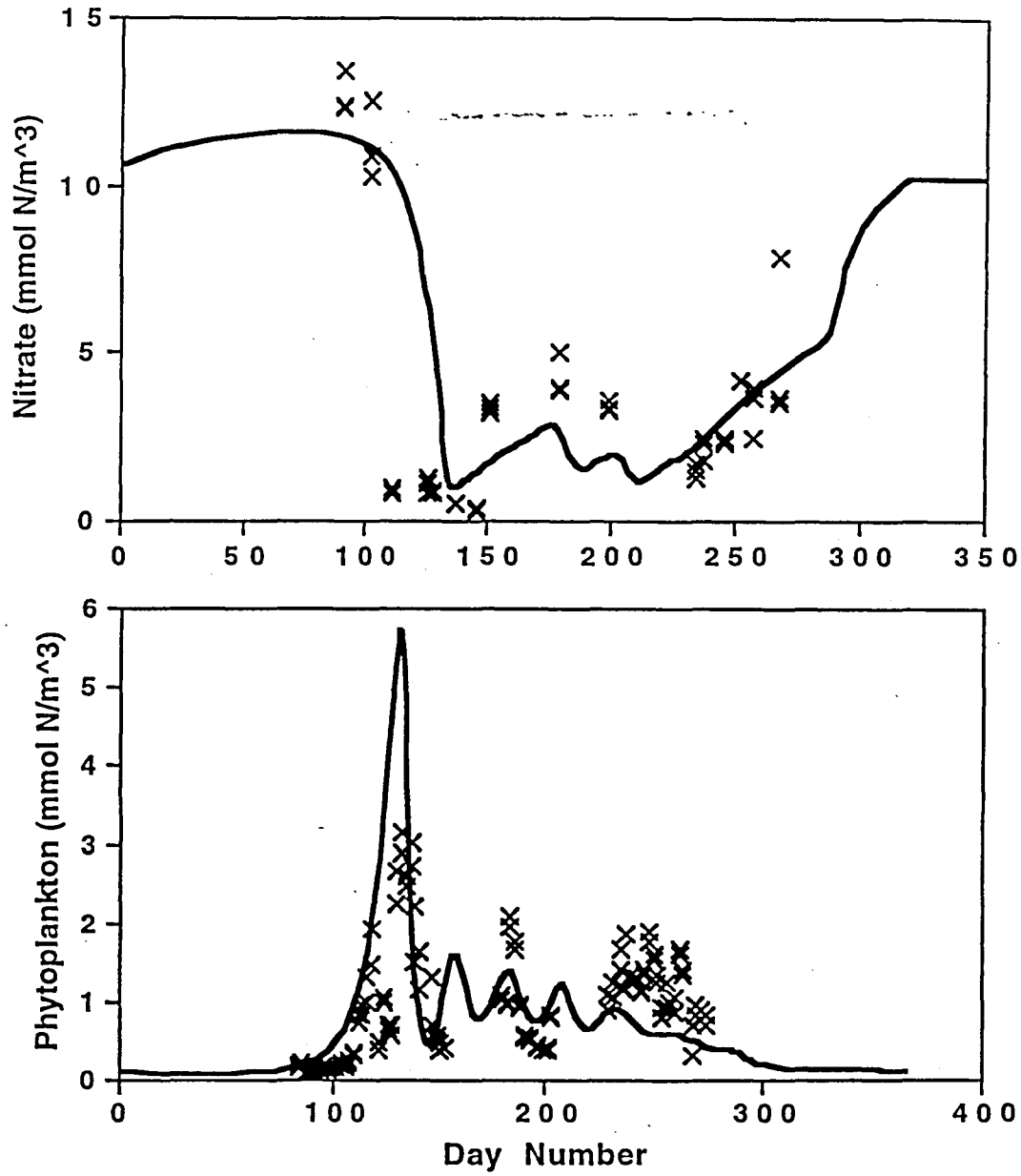


Fig. 9. Fit of the five-compartment model to nitrate (top) and phytoplankton (bottom) observations at OWS India.

The question now arises as to whether the model can reproduce both types of annual cycle with the same model parameter set. To test this we calculated the average value of the ecosystem model parameters obtained from the two separate optimisations. These averaged ecosystem parameter values were then used in conjunction with the different environmental parameters obtained for each station (i.e., nitrate gradient, mixed layer depths, cloudiness, and mixing rate). It was found that the two simulations obtained gave good fits to the seasonal cycles of chlorophyll and nitrate at both stations. These results

give us encouragement that robust ecosystem models capable of modelling different areas of the ocean with the same parameter set can be developed.

References

Brock, T.D. 1981 Calculating solar radiation for ecological studies. *Ecol. Modell.* 14,1-19

Ducklow, H.W. & Harris, R.P. 1993 Introduction to the JGOFS North Atlantic Bloom Experiment. *Deep-Sea Res. II* 40, 1-8.

Evans, G.T. & Parslow, J.S. 1985. A model of annual plankton cycles. *Biol Oceanogr.* 3,327-347

Fasham, M.J.R. 1993 Modelling the marine biota. In The global carbon cycle (ed. M. Heimann), pp. 457-504. Heidelberg: Springer-Verlag.

Fasham, M.J.R. 1995. Variations in the seasonal cycle of biological production in subarctic oceans: A model sensitivity analysis. *Deep-Sea Res.*, 42, 1111-1149

Fasham, M.J.R., Ducklow, H.W. & McKelvie, S.M. 1990 A nitrogen-based model of plankton dynamics in the oceanic mixed layer. *J. Mar. Res.* 48, 591-639.

Fasham, M.J.R. & Evans, G.T, 1995. The use of optimization techniques to model marine ecosystem dynamics at the JGOFS station at 47°N 20°W. Phil. Trans. R. Soc. Lond. B. 203-209

Frost, B.W. 1987 Grazing control of phytoplankton stock in the subarctic Pacific: a model assessing the role of mesozooplankton, particularly the large calanoid copepods, *Neocalanus* spp. *Mar. Ecol. Progr. Series* 39, 49-68.

Frost, B.W. 1993 A modelling study of processes regulating plankton standing stock and production in the open subarctic Pacific. *Progr. Oceanogr.* 32, 17-57.

Hurtt, G C & Armstrong, R A. 1996. A pelagic ecosystem model calibrated with BATS data. *Deep-Sea Res.* II, 43, 653-683.

R. & Stienen, C. 1993 Plankton succession and carbon cycling at 47°N 20°W during the North Atlantic Boom Experiment. *Deep-Sea Res. II* 40, 91-114.

Levitus, S. 1982 Climatological atlas of the world ocean. *NOAA Professional Paper 13* ,Washington: US Govt Printing Office.

McGillicuddy, D.J., McCarthy, J.J. & Robinson, A.R. 1995 Coupled physical and biological modeling of the spring bloom in the North Atlantic (I): Model formulation and one dimensional bloom processes. *Deep-Sea Res.*, in press.

Martin, J.H., Fitzwater, S.E., Gordon, R.M., Hunter, C.N. & Tanner, S.J. 1993 Iron, primary production and carbon-nitrogen flux studies during the North Atlantic Bloom Experiment. *Deep-Sea Res. II* 40, 115-134

Miller, C. B., 1993. Pelagic processes in the Subarctic Pacific. Prog. Oceanogr. 32, 1-15

Press, W.H., Teukolsky, S.A., Vetterling, W.T. & Flannery, B.P. 1992 *Numerical recipes in C.* Cambridge University Press.

Robinson, A.R., McGillicuddy, D.J., Calman, J., Ducklow, H.W., Fasham, M.J.R., Hoge, F.E., Leslie, W.G., McCarthy, J.J., Podewski, S., Porter, D.L., Saure, G. & Yoder, J.A. 1993 Mesoscale and upper ocean variabilities during the 1989 JGOFS bloom study. *Deep-Sea Res. II* **40**, 9-36.

Ryabchenko, V.A., Fasham, M.J.R., Kagan, B.A. And Popova, E.E., 1996. What causes oscillations in ecosystem models of the marine mixed layer? *J. Mar. Sys.*, in press

Sieracki, M.E., Verity, P.G. & Stoecker, D.K. 1993 Plankton community response during the 1989 North Atlantic spring bloom. *Deep-Sea Res. II* **40**, 213-226.

Steele, J.H. & Henderson, E.W. 1992 The role of predation in plankton models. *J. Plank. Res.* **14**,157-172.

Steele, J.H. & Henderson, E.W. 1993 the significance of interannual variability. In *Towards a model of ocean biogeochemical processes* (ed. G.T. Evans & M.J.R. Fasham), pp. 237-260. Heidelberg: Springer-Verlag.