



Contents lists available at ScienceDirect

## Progress in Oceanography

journal homepage: [www.elsevier.com/locate/pocean](http://www.elsevier.com/locate/pocean)

## Application of an automatic approach to calibrate the NEMURO nutrient–phytoplankton–zooplankton food web model in the Oyashio region

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## ARTICLE INFO

## Article history:

Available online 8 October 2010

## ABSTRACT

The Oyashio region in the western North Pacific supports high biological productivity and has been well monitored. We applied the NEMURO (North Pacific Ecosystem Model for Understanding Regional Oceanography) model to simulate the nutrients, phytoplankton, and zooplankton dynamics. Determination of parameters values is very important, yet ad hoc calibration methods are often used. We used the automatic calibration software PEST (model-independent Parameter ESTimation), which has been used previously with NEMURO but in a system without ontogenetic vertical migration of the large zooplankton functional group. Determining the performance of PEST with vertical migration, and obtaining a set of realistic parameter values for the Oyashio, will likely be useful in future applications of NEMURO. Five identical twin simulation experiments were performed with the one-box version of NEMURO. The experiments differed in whether monthly snapshot or averaged state variables were used, in whether state variables were model functional groups or were aggregated (total phytoplankton, small plus large zooplankton), and in whether vertical migration of large zooplankton was included or not. We then applied NEMURO to monthly climatological field data covering 1 year for the Oyashio, and compared model fits and parameter values between PEST-determined estimates and values used in previous applications to the Oyashio region that relied on ad hoc calibration. We substituted the PEST and ad hoc calibrated parameter values into a 3-D version of NEMURO for the western North Pacific, and compared the two sets of spatial maps of chlorophyll-*a* with satellite-derived data. The identical twin experiments demonstrated that PEST could recover the known model parameter values when vertical migration was included, and that over-fitting can occur as a result of slight differences in the values of the state variables. PEST recovered known parameter values when using monthly snapshots of aggregated state variables, but estimated a different set of parameters with monthly averaged values. Both sets of parameters resulted in good fits of the model to the simulated data. Disaggregating the variables provided to PEST into functional groups did not solve the over-fitting problem, and including vertical migration seemed to amplify the problem. When we used the climatological field data, simulated values with PEST-estimated parameters were closer to these field data than with the previously determined ad hoc set of parameter values. When these same PEST and ad hoc sets of parameter values were substituted into 3-D-NEMURO (without vertical migration), the PEST-estimated parameter values generated spatial maps that were similar to the satellite data for the Kuroshio Extension during January and March and for the subarctic ocean from May to November. With non-linear problems, such as vertical migration, PEST should be used with caution because parameter estimates can be sensitive to how the data are prepared and to the values used for the searching parameters of PEST. We recommend the usage of PEST, or other

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parameter optimization methods, to generate first-order parameter estimates for simulating specific systems and for insertion into 2-D and 3-D models. The parameter estimates that are generated are useful, and the inconsistencies between simulated values and the available field data provide valuable information on model behavior and the dynamics of the ecosystem.

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## 1. Introduction

The Oyashio is the subarctic western boundary current of the western North Pacific, and supports high biological production. The subarctic gyre is composed of two major gyres: the western subarctic gyre and the Alaskan gyre (Favorite et al., 1976; Qiu, 2002; Pickart et al., 2009) (Fig. 1). The Oyashio is part of the western subarctic gyre, and is a continuation of the East Kamchatka Current and fed by waters from the western subarctic gyre and from the Sea of Okhotsk (Shimizu et al., 2001). The Oyashio flows southward along Hokkaido Island and Honshu Island of Japan, and then turns and flows eastward with meanders. The meander crests (to the south) are called the First and Second Branches of the Oyashio according to their proximity to land (Kawai, 1972). The eastward flowing Oyashio becomes the Subarctic Front (Oyashio Front), which is a distinctive temperature front, and then the Subarctic Current or West Wind Drift (Sverdrup et al., 1942; Dodimead et al., 1963). While a portion of the Subarctic Current turns northward and becomes the western subarctic gyre, the remaining portion continues to flow eastward until it bifurcates to form the northward-flowing Alaska Current and the southward-flowing California Current (Sverdrup et al., 1942; Chelton and Davis, 1982). The Alaska Current flows along the west coast of North America and continues into the southwestward flowing Alaskan Stream, which is the western boundary current of the Alaskan gyre (Reed and Stabeno, 1989).

In the western subarctic gyre, high nutrients result in high primary productivity. Cyclonic wind stress curl causes upward motion and an influx of nutrient-rich water into the euphotic zone (i.e., Ekman pumping). Additionally, deep vertical convection in the winter and strong tidal mixing along the Kuril Islands also bring nutrient-rich water into the surface layer (Nakamura et al., 2006; Sarmiento et al., 2004). Thus, Oyashio water is low-salinity, cool, and nutrient-rich. This supports high primary productivity, and a strong spring phytoplankton bloom occurs because of seasonal stratification. Annual primary production was reported as 146–301 gC m<sup>-2</sup> yr<sup>-1</sup> (Kasai et al., 2001; Takahashi et al., 2008), and the maximum chlorophyll-*a* concentration can exceed 40 mg m<sup>-3</sup> (Kasai et al., 1997).

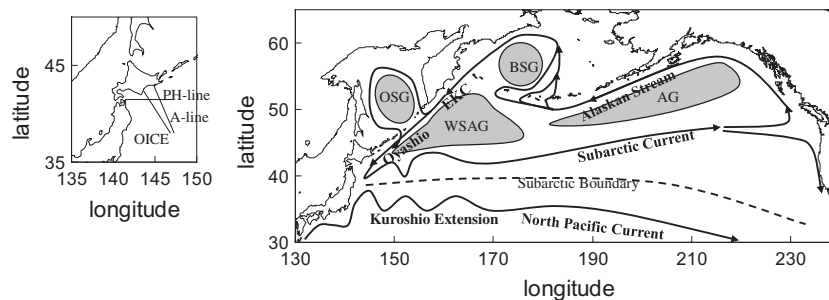
The high primary production in the Oyashio, in turn, supports high zooplankton production that also shows strong seasonal variation (Saito et al., 2002; Takahashi et al., 2008). Dominant zooplankton in the Oyashio region are herbivorous calanoid copepods, including three species of *Neocalanus* (*Neocalanus flemingeri*,

*Neocalanus plumchrus*, and *Neocalanus cristatus*) and one species of *Eucalanus* (*Eucalanus bungii*) (Tsuda et al., 1999, 2004). These dominant zooplankton species have 1–2 year life cycles that involve ontogenetic vertical migration. Typical vertical migration involves staying in the epipelagic layer during spring to summer for feeding and then descending to the mesopelagic layer during autumn to winter. Although the timing of vertical migration depends on the species, the three *Neocalanus* species are spawned in deep waters without feeding, using organic matter stored during their epipelagic-inhabiting period and their offspring (nauplii) ascend to the epipelagic layer for foraging. Since the timing of vertical migration is often synchronized in the population (Saito et al., 2009), the downward migration of the dominant zooplankton means a sudden decline in zooplankton biomass from the epipelagic zone and the upward migration means a sudden increase.

*Neocalanus* are important food for many pelagic fish, including commercially important species such as Pacific saury *Cololabis saira*, Japanese sardine *Sardinops melanostictus*, and Japanese anchovy *Engraulis japonicus*, which migrate into the Oyashio region from warm water regions during summer and autumn (Odate, 1994; Ito et al., 2004a). However, interannual to decadal variability of transport in the Oyashio is comparable to its seasonal variability, and this interannual variability affects the water properties and mixed layer depth of the Oyashio, with cascading effects on biological productivity (Qiu, 2002; Ito et al., 2004b). Moreover, the transport of *Calanus* from the First Branch of the Oyashio is an important source of organic carbon in the mixed water region (Shimizu et al., 2009), which is located between the Oyashio Front and the Kuroshio Extension Front.

The Oyashio has been well studied, and several long-term observational transects are maintained. The Fishery Agency and prefectural fisheries observatory of Japan have been conducting monthly hydrographic measurements since 1965. Long-term transects include the PH-line on 41.5°N (Takatani et al., 2007), the A-line which is southeastward from Hokkaido Island and crosses the Oyashio (Saito et al., 2002), and the OICE (Oyashio Intensive observation line off Cape Erimo) along the ground track of a satellite altimeter (TOPEX/POSEIDON) (Ito et al., 2004b) (Fig. 1).

While many data are available related to the physical, chemical, and biological aspects of the Oyashio, there is only limited information about the flows among the nutrients and lower trophic level biota and how the lower trophic levels might respond to variations in environmental conditions (e.g. Shinada et al., 2000; Takahashi et al., 2008, 2009). Such information is difficult to obtain



**Fig. 1.** Repeated observation lines in the Oyashio region (left) and schematic diagrams of circulation in the subarctic North Pacific (right). WSAG: western subarctic gyre, AG: Alaskan gyre, BSG: Bering Sea gyre, OSG: Okhotsk Sea gyre, EKC: East Kamchatka Current. The schematics were redrawn from Sverdrup et al. (1942), Dodimead et al. (1963) and Favorite et al. (1976).

with field data alone because observations are discrete in time and limited spatially. Nutrient–phytoplankton–zooplankton (NPZ) modeling offers a complementary approach that can utilize the field data and attempt to simulate the energy flows among key biota. NPZ models have been widely used in marine ecosystem analysis (Hood et al., 2006; Le Quere et al., 2005). Energy flows in these NPZ models are largely determined by the parameter values used. In this paper, we applied the NEMURO (North Pacific Ecosystem Model for Understanding Regional Oceanography; Kishi et al., 2007) NPZ model to the Oyashio region. We focus on automatic calibration as a means of objectively determining the parameter values of NEMURO.

NEMURO was developed as a unified NPZ model designed to be flexible and general enough to be applied to a variety of locations in the North Pacific (Kishi et al., 2007). NEMURO was developed as part of a GLOBEC (Global Ocean Ecosystem Dynamics) regional program, “Climate Change and Carrying Capacity” (CCCC), that was a joint program with PICES (North Pacific Marine Science Organization). NEMURO has been applied to the Oyashio region and other regions (Werner et al., 2007). However, like other NPZ models, NEMURO has many parameters and it is impossible to *a priori* estimate values of all of the model parameters from experiments and observations. Therefore, the calibration of NEMURO to site-specific data is an important issue.

Many NPZ models are calibrated by manually adjusting parameter values in a trial-and-error approach (i.e., ad hoc) until model predictions agree sufficiently with the observed data (Rose et al., 2007). With ad hoc calibration, we do not know if the parameter estimates obtained are optimal and how model responses to changed conditions are influenced by the particular set of parameter values that were obtained. Kuroda and Kishi (2004) applied a variational adjoint method to NEMURO and estimated optimal parameter values by assimilating observational data. They showed the feasibility of using variational adjoint methods with NEMURO and illustrated how it could improve model performance. Friedrichs et al. (2007) applied variational adjoint methods to a 1-D version of NEMURO. While variational adjoint methods are powerful and commonly used (Lawson et al., 1995, 1996; Matear, 1995; Robinson and Lermusiaux, 2002; Friedrichs et al., 2007), they often require significant additional model coding. Recently, there have been efforts to develop automatic coding systems to help in the application of variational adjoint methods (e.g., Heimbach et al., 2005). There are also several other methods that have been used to estimate optimal model parameters, including simulated annealing (Matear, 1995) and genetic algorithms (Ward et al., 2010). All of these methods automatically search the parameter space trying to minimize the difference between model-simulated values and observations.

In this paper we investigate an automatic calibration software package, model-independent Parameter ESTimation or PEST (Doherty, 2004; Doherty and Johnston, 2003), which is widely used in groundwater and other modeling applications, and has the distinct advantage of operating with minimal changes to the model code itself. Rose et al. (2007) first applied PEST to estimate optimal parameters of NEMURO for the West Coast Vancouver Island and demonstrated that such estimation schemes can be helpful with model development and application. However, Rose et al.'s (2007) version of NEMURO did not include ontogenetic vertical migration of the large zooplankton group because of the shallowness of their location. Vertical migration is important elsewhere and has been included in many other NEMURO applications (Werner et al., 2007).

In this paper, we used NEMURO, with and without vertical ontogenetic migration of large zooplankton, to investigate how vertical migration would affect parameter estimation by PEST. We applied a zero-dimensional one-box version of NEMURO to

the Oyashio region because of the importance of this region to plankton and fish production and because of the availability of long-term observational data. Determining the performance of PEST with vertical migration and obtaining a set of realistic parameter values for the Oyashio will likely be useful in future applications of NEMURO. Five identical twin simulation experiments were performed that varied the mix of model state variables included in the minimization and whether or not vertical migration of large zooplankton was included. We then applied NEMURO to monthly climatological field data covering 1 year for the Oyashio, and compared model fits and parameter values between PEST-determined estimates and values used in previous application to the Oyashio region that relied on ad hoc calibration. We also substituted the PEST and ad hoc calibrated parameter values into a 3-D version of NEMURO for the western North Pacific, and compared spatial maps of chlorophyll-*a* generated using the two parameter sets with satellite-derived data. We discuss some of the difficulties of using PEST when vertical migration of biota occurs, possible confounding of parameter estimation due to model simplifications, and the realism of parameter estimates obtained for the Oyashio relative to available field and laboratory data and relative to the results obtained by a similar analysis for a coastal area in the eastern North Pacific. Finally, we conclude with a suggested approach for calibrating NEMURO to new locations.

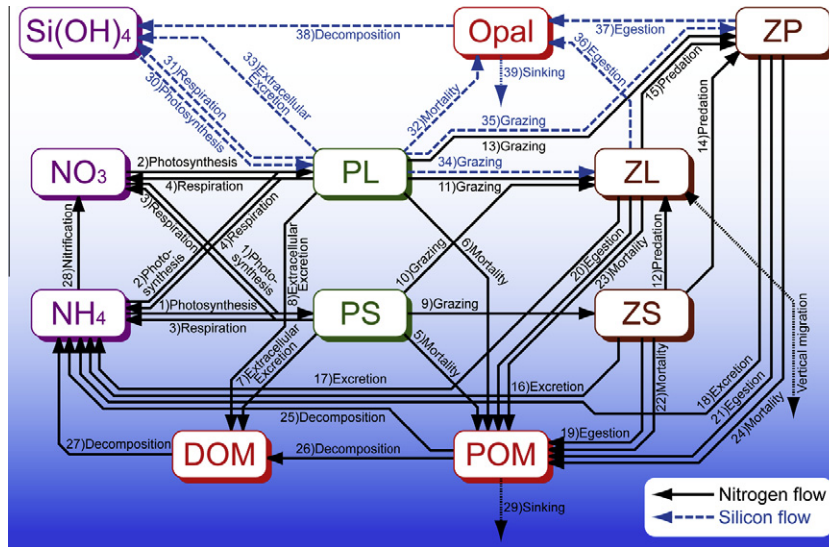
## 2. Materials and methods

### 2.1. One-box and 3-D-NEMURO models

We used both a one-box NEMURO version and a version with NEMURO imbedded in a 3-D hydrodynamic model (3-D-NEMURO). Both versions used the same NEMURO model for the NPZ dynamics (Fig. 2), which is described in detail in Kishi et al. (2007). The one-box and 3-D versions differed in how their forcing functions to NEMURO were determined, and in the inclusion of advective transport in the 3-D version. Forcing functions were specified for the one-box version, whereas forcing variables were dynamically generated in space and time by the physical model in the 3-D version.

NEMURO has eleven state variables: nitrate ( $\text{NO}_3$ ), ammonium ( $\text{NH}_4$ ), silicic acid ( $\text{Si}(\text{OH})_4$ ), small phytoplankton (PS), large phytoplankton or diatoms (PL), small zooplankton (ZS), large zooplankton (ZL), predatory zooplankton (ZP), non-living particulate organic nitrogen (PON), particulate organic silicon (Opal), and dissolved organic matter (DON). There are eleven coupled ordinary differential equations, which describe the rate of change of each state variable. This system of differential equations was solved using an Euler scheme with a 1 h time step. The units of all state variables were calculated as  $\mu\text{molN L}^{-1}$  for the nitrogen cycle and  $\mu\text{molSi L}^{-1}$  for the silicon cycle, and a constant uptake ratio of nitrogen to silicon was assumed for the diatoms ( $R_{\text{SiN}}$ ).

The differential equations describing the rate of change of the two phytoplankton groups were expressed as photosynthesis rate minus the loss rates due to respiration, mortality, extracellular excretion, and grazing by zooplankton. Photosynthesis was assumed to be a function of phytoplankton concentration, temperature, nutrient concentration, and intensity of light. Nutrient limitation of photosynthesis was determined by a Michaelis–Menten formula plus a process related to uptake inhibition of nitrate in the presence of ammonium (Wroblewski, 1977). Light limitation was computed using a light inhibition function based on the incident solar radiation (Steele, 1962) and phytoplankton self-shading. A Q10 function was used to determine the temperature effect on photosynthesis. Maximum photosynthetic rate ( $V_{\text{max}}$ ), which is photosynthetic rate at 0 °C with no limitation due to nutrients and light, was used to express the maximum



**Fig. 2.** Schematic flow chart of NEMURO (after Kishi et al., 2007). Solid black arrows indicate nitrogen flows and dashed blue arrows indicate silicon flows. Dotted black arrows represent the exchange or sinking of material between the modeled box and below the mixed layer depth.

magnitude of photosynthesis possible. Respiration, mortality, and zooplankton grazing were all temperature-dependent based on Q10 functions.

The differential equations for the three types of zooplankton were expressed as their growth from grazing of phytoplankton and/or zooplankton minus predation by upper-trophic-level zooplankton, mortality, excretion, and egestion. Zooplankton grazing was assumed to depend on plankton prey concentration based on an Ivlev function, which assumed no grazing when plankton prey concentration was lower than a critical concentration. Maximum grazing rate ( $Gr_{max}$ ), which is grazing rate at 0 °C with no limitation of prey, was used to express the maximum magnitude of grazing possible. Ontogenetic vertical migration was assumed, such that all ZL in the mixed layer moved out of the model box (i.e., went below the mixed layer depth, MLD) on September 1, only 20% of the ZL survived until the next spring and these migrated up to the simulated box on April 1.

The one-box version of NEMURO required specification of the daily forcing functions of temperature, incident solar radiation, MLD, and nutrient flux from below the MLD into the simulated box. The forcing functions were idealized annual cycles that were repeated every year in the simulations. Daily water temperature ( $T$ , °C) and daily incident solar radiation at the surface ( $L_0$ ,  $\text{ly min}^{-1}$ ) in the simulated surface box were derived from climatological data in the Oyashio region:

$$T = 9.0 + 7.0 * \cos(2.0 * \pi * (\text{jday}/365 - 0.67)), \text{ and}$$

$$L_0 = 0.1 * (1.05 + 0.32 * \cos(2.0 * \pi * (\text{jday}/365 - 0.48))),$$

where jday is Julian day (Jan 1 = 1, Jan 2 = 2, etc.) (Fig. 3a). The MLD (i.e., thickness of the simulated surface box in meters) was calculated each day by solving the following differential equations through time beginning with an initial value of 30 m on January 1 in year 1:

$$d\text{MLD}/dt = (20 - \text{MLD})/(30 * 86,400) \text{ for March 17th} \\ \text{–September 27th,}$$

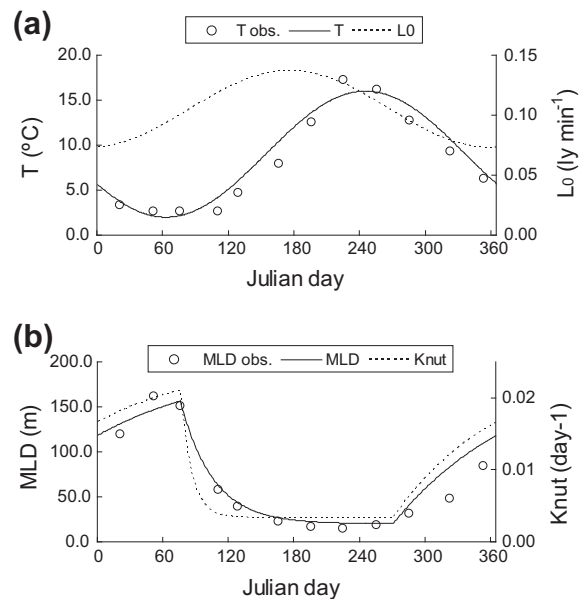
$$d\text{MLD}/dt = (200 - \text{MLD})/(120 * 86,400) \text{ for September 28th} \\ \text{–March 16th,}$$

where  $t$  is time in seconds and 86,400 is the number of seconds in 1 day. We integrated the one-box version of the model for 6 years, and state variables showed consistent seasonal dynamics by the

second year. The seasonal variation of the simulated MLD reasonably captures the observed seasonal variation: MLD reached about 20 m during March 17 to September 27 and then slowly increased to 200 m during September 28 to March 16 (Fig. 3b). The exchange parameter ( $K_{nut}$ ,  $\text{s}^{-1}$ ), which is the inverse of the time scale of exchange of nutrients between the simulated box and the deeper waters below the MLD, was also computed from a differential equation:

$$dK_{nut}/dt = (1/(300 * 86,400) - K_{nut})/(10 * 86,400) \text{ for March 17th} \\ \text{–September 27th,}$$

$$dK_{nut}/dt = (1/(40 * 86,400) - K_{nut})/(100 * 86,400) \text{ for September 28th} \\ \text{–March 16th.}$$



**Fig. 3.** (a) Water temperature (solid line) and incident solar radiation at the surface (dotted line) as forcing functions of the one-box version of NEMURO. Climatological water temperature of the mixed layer in the Oyashio region (white circles) is also shown. (b) Resulting MLD (solid line) and exchange parameter  $K_{nut}$  (dotted line) in the one-box model. The unit of  $K_{nut}$  was converted to  $\text{day}^{-1}$ . Climatological MLD in the Oyashio region (white circles) is also shown.



$K_{\text{nut}}$  started at the equivalent of  $1/(100 \text{ days})$  on January 1 in year 1. In the steady state,  $K_{\text{nut}}$  rapidly decreased to about  $1/300 \text{ day}^{-1}$  after March 17 and stayed there until September 27, after which  $K_{\text{nut}}$  slowly increased toward  $1/40 \text{ day}^{-1}$  between September 28 and March 16 (Fig. 3b). The flux of nutrients from below the MLD was then computed each day as  $K_{\text{nut}}$  times specified nitrate ( $\text{NO}_{3\text{b}}-\text{NO}_3$ ) and silicic acid ( $\text{Si}(\text{OH})_{4\text{b}}-\text{Si}(\text{OH})_4$ ) concentrations, where  $\text{NO}_{3\text{b}}$  and  $\text{Si}(\text{OH})_{4\text{b}}$  are the deep waters values of nitrate and silicic acid, respectively. We used  $20.0 \mu\text{molN L}^{-1}$  and  $35.0 \mu\text{molSi L}^{-1}$  for  $\text{NO}_{3\text{b}}$  and  $\text{Si}(\text{OH})_{4\text{b}}$ , respectively, which were derived from the climatology. The flux of nitrate and silicic acid into the simulated box increased during the winter and decreased during the summer.

The 3-D-NEMURO version was a previous implementation for the western North Pacific and is described in detail by Hashioka et al. (2009). Physical fields were calculated by an ocean-atmosphere coupled model, the Model for Interdisciplinary Research On Climate (MIROC) version 3.2, with external forcing of solar and volcanic activity, greenhouse gas concentrations, various aerosol emissions, and land-use estimated as 1900 (preindustrial) conditions (Sakamoto et al., 2005). The MIROC model used a horizontal grid-spacing of  $0.28^\circ$  (zonally) by  $0.19^\circ$  (meridionally), and covered the top 1500 m in the western North Pacific (about  $110^\circ\text{E}-180^\circ$ ,  $10-60^\circ\text{N}$ ). The physical field of MIROC, after 109 years of spin-up, simulated an additional 46 years of the 1900 conditions. Climatological data of WOA2005 were used to specify the initial conditions of  $\text{NO}_3$  and  $\text{Si}(\text{OH})_4$ . The ammonium concentration was set to  $0.5 \mu\text{molN L}^{-1}$ , PON, DON and Opal were set to  $0.0 \mu\text{molN L}^{-1}$  (or  $\mu\text{molSi L}^{-1}$ ), and other compartments were set to  $0.5 \mu\text{molN L}^{-1}$  (or  $\mu\text{molSi L}^{-1}$ ). The ontogenetic vertical migration of ZL was eliminated in 3-D-NEMURO because identical twin experiments showed that PEST-based parameter estimation was more robust without vertical migration (shown below). 3-D-NEMURO was integrated for 3 years using repeated values of the final year (year 46) of the physical fields, and 3-D-NEMURO results in the third year were used in the analysis.

## 2.2. PEST software

We used the PEST software (Doherty, 2004) to automatically calibrate the one-box NEMURO. An advantage of PEST is that it operates externally to the NEMURO source code. PEST and the model communicate via input and output files. PEST automatically runs the model, which reads in parameter values from an input file and writes model results to an output file. PEST then reads the model output file and calculates the squared error between observations and model predictions and adjusts values of parameters to minimize the weighted sum of squared deviations. PEST then writes a new NEMURO input file, the model is run, and the process is repeated many times.

PEST determines the adjustment to the parameters each time in a series of steps using a variation of the Gauss–Marquardt–

Levenberg algorithm (Doherty, 2004). PEST first approximates the relationship between observations and model parameters using a Taylor series expansion, which involves the Jacobian matrix (the matrix of partial derivatives of observations with respect to parameters). PEST computes the partial derivatives of the Jacobian matrix using central differences; parameters are varied small amounts from the current set of values, the model rerun, and the derivatives computed. New values of parameters are then determined (parameter update vector) using the Marquardt parameter (denoted  $\lambda$ ), which is based on the gradient of the objective function (derivative of the objective function with respect to parameters). PEST stops searching when the objective function does not go lower over several iterations, when the changes in parameters dictated by the update vector are very small, or when the number of iterations or other internal limits on calculations are triggered. The final updated model parameters can be considered as optimal in the sense that they result in the minimization of the squared differences between observations and model predictions.

For all of our analyses, we specified broad upper ( $10^{10}$ ) and lower (0.05) limits to parameter values, and used default values of all parameters in PEST that control its searching behavior of the parameter space, except three parameters (NPHINORED, RELPARMAX and FACPARMAX). The modification and definition of the three PEST parameter values will be explained in the next subsection.

## 2.3. Identical twin experiments using the one-box model

We conducted a series of identical twin experiments with the one-box version of NEMURO using a similar approach as used by Rose et al. (2007). Daily forcing functions were used and repeated for 6 years using known NEMURO parameter values. We used the NEMURO parameter values reported in Kishi et al. (2007), who calibrated NEMURO to field data at station A7 using an ad hoc (fit by trial and error) approach. We refer to the parameter values reported by Kishi et al. (2007) as the nominal values. Station A7 is sometimes in the Oyashio and other times reflects conditions of the mixed water region. Monthly snapshot data (on the middle day of each month) or monthly averaged data of nutrient concentrations and phytoplankton and zooplankton group densities in year 6 were treated as the virtual data. The two phytoplankton maximum photosynthetic rate parameters ( $V_{\text{maxS}}$  and  $V_{\text{maxL}}$ ) and the seven zooplankton maximum grazing rate parameters ( $G_{\text{max}}$ ) were then set to  $0.5 \text{ day}^{-1}$  and the uptake ratio of nitrogen to silicon ( $R_{\text{SiN}}$ ) was set to 2.0 as starting values for PEST, and PEST was used to see if we could recover the original (nominal) values of the ten parameters (Table 1). We focused on the photosynthetic and grazing rate parameters because these have been shown to be very important in controlling phytoplankton and zooplankton dynamics in NEMURO. Yoshie et al. (2007) investigated parameter sensitivity of NEMURO using Monte Carlo simulations and one parameter-at-a-time methods and showed that the maximum photosynthetic

**Table 1**  
NEMURO model parameters that were varied as part of the PEST automatic calibration.

Parameters	Definitions	Units
$V_{\text{maxS}}$	Maximum photosynthetic rate at $0^\circ\text{C}$ of small phytoplankton	$\text{day}^{-1}$
$V_{\text{maxL}}$	Maximum photosynthetic rate at $0^\circ\text{C}$ of large phytoplankton	$\text{day}^{-1}$
$G_{\text{maxZS\_PS}}$	Maximum grazing rate at $0^\circ\text{C}$ of small zooplankton on small phytoplankton	$\text{day}^{-1}$
$G_{\text{maxZL\_PS}}$	Maximum grazing rate at $0^\circ\text{C}$ of large zooplankton on small phytoplankton	$\text{day}^{-1}$
$G_{\text{maxZL\_PL}}$	Maximum grazing rate at $0^\circ\text{C}$ of large zooplankton on large phytoplankton	$\text{day}^{-1}$
$G_{\text{maxZL\_ZS}}$	Maximum grazing rate at $0^\circ\text{C}$ of large zooplankton on small zooplankton	$\text{day}^{-1}$
$G_{\text{maxZP\_PL}}$	Maximum grazing rate at $0^\circ\text{C}$ of predatory zooplankton on large phytoplankton	$\text{day}^{-1}$
$G_{\text{maxZP\_ZS}}$	Maximum grazing rate at $0^\circ\text{C}$ of predatory zooplankton on small zooplankton	$\text{day}^{-1}$
$G_{\text{maxZP\_ZL}}$	Maximum grazing rate at $0^\circ\text{C}$ of predatory zooplankton on large zooplankton	$\text{day}^{-1}$
$R_{\text{SiN}}$	Si:N ratio of large phytoplankton	No dimension

**Table 2**

Five identical twin experiments that differed in the aggregation of the state variables, in whether the values of the monthly state variables were snapshots or averages, and in whether vertical migration was included.

Experiments	Predicted variables	Type of predicted variables	Ontogenetic migration
Exp-1	NO <sub>3</sub> , Si(OH) <sub>4</sub> , PS + PL, ZS + ZL	Monthly snapshot	Included
Exp-2	NO <sub>3</sub> , Si(OH) <sub>4</sub> , PS + PL, ZS + ZL	Monthly average	Included
Exp-3	NO <sub>3</sub> , Si(OH) <sub>4</sub> , PS + PL, ZS + ZL	Monthly snapshot	Excluded
Exp-4	NO <sub>3</sub> , Si(OH) <sub>4</sub> , PS + PL, ZS + ZL	Monthly average	Excluded
Exp-5	NO <sub>3</sub> , Si(OH) <sub>4</sub> , PS, PL, ZS, ZL	Monthly average	Excluded

rate and maximum grazing rate parameters were consistently ranked as important in affecting phytoplankton and zooplankton biomass at Station A7.  $R_{SiN}$  was included because of strong silicon limitation at Station A7 and other western North Pacific locations (Fujii et al., 2007), and because of its importance in NEMURO applied to Station KNOT (Fujii et al., 2002). Additionally, it was also constantly ranked as important in affecting Si(OH)<sub>4</sub> in the sensitivity analyses reported by Yoshie et al. (2007).

We conducted five separate identical twin experiments that differed in how the monthly virtual data were aggregated and whether vertical migration was included or not (Table 2). In experiment 1 (Exp-1), we used monthly snapshots of NO<sub>3</sub>, Si(OH)<sub>4</sub>, the sum of the two phytoplankton groups, and the sum of small and large zooplankton. The summed phytoplankton mimics total chlorophyll-*a*, which is commonly measured in field surveys. The sampling efficiency of the small and large zooplankton groups (ZS and ZL) is better than for the predatory zooplankton group, and so when total zooplankton data are available, it more closely corresponds to the sum of small and large zooplankton. NH<sub>4</sub> was not used because it is difficult to measure in field monitoring. In experiment 2 (Exp-2), we used the same variables but used monthly averaged values instead of monthly snapshot values. Snapshot values differed slightly from monthly averages, so comparison of experiments 1 and 2 is a test of the effect of small differences in data accuracy on the model parameter estimation. Experiment 3 (Exp-3) was identical to Exp-1, except that large zooplankton were not allowed to vertically migrate. Experiment 4 was the same as Exp-2 but again the large zooplankton were not allowed to vertically migrate. In experiment 5 (Exp-5), the small and large phytoplankton and zooplankton groups were treated separately to test the influence of data availability (i.e., specific functional groups versus aggregated) on model parameter estimation. Because of differences in the variation among the monthly values of nutrients and plankton densities, we normalized the monthly time series of each variable by subtracting each value by its overall annual mean and dividing by its standard deviation. In this way, seasonal variation in some variables was not overshadowed by wider seasonal variation in other variables. PEST was then applied to minimize the squared difference between the normalized data and normalized model outputs.

For each experiment, we compared the PEST-estimated parameter values with the original (nominal) values that generated the virtual data. We also compared time series plots of the monthly virtual data with two sets of simulated values. The first set of simulated values was based on using the initial values of parameters that PEST started with (maximum photosynthesis and grazing rates set to 0.5 day<sup>-1</sup> and  $R_{SiN}$  set to 2.0), and the second set was based on using the final PEST parameter values. We wanted to see whether the PEST-estimated parameter values generated a simulation that provided a reasonably good fit to the virtual data and how much they improved the fit over that based on arbitrary values.

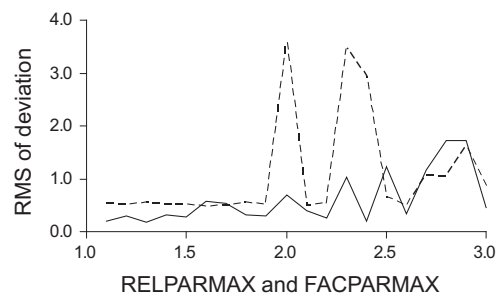
We also summarized the differences between two sets of estimated parameter values or two sets of predicted state variables by computing the root-mean-square (RMS) between the values

(summed over parameters or over months and state variables). RMS can be differentially influenced by the magnitude of the variables included. With the NEMURO model parameters, the units of  $R_{SiN}$  were different from the other parameters, but we ignored this because we used RMS as a rough measure of differences. For the state variables, all variables were reported in  $\mu\text{molN L}^{-1}$ .

In advance of conducting the identical twin experiments, we investigated how PEST parameters influenced the performance of PEST. As a result of these initial analyses, we modified three parameters of PEST from their default values: NPHINORED, RELPARMAX and FACPARMAX. NPHINORED is the maximum number of iterations allowed when the objective function does not decrease between subsequent evaluations. The default value in PEST was 3, but we found better performance by using a value of 5, which permitted more iterations as PEST approached the global minimum before stopping the parameter searching. RELPARMAX is the maximum relative change that a parameter is allowed to undergo between optimization iterations, and FACPARMAX is the maximum change in its value that a parameter is allowed to undergo (Doherty, 2004). For highly non-linear problems, these values are best set to low values, which increases the number of iterations (i.e., model runs) required for fitting. We varied the RELPARMAX and FACPARMAX from 1.1 to 2.0 using Exp-4 conditions, and compared the RMS values of NEMURO parameter values and associated state variable values between those determined by PEST versus the original values (Fig. 4). Based on these preliminary simulations, we determined that RELPARMAX and FACPARMAX set to 1.3 were needed. Higher values of the two PEST parameters caused estimated parameter values to diverge from the original (known) values. In all experiments, we used the modified values for NPHINORED, RELPARMAX, and FACPARMAX.

#### 2.4. Calibration of one-box model using field data

We used field data and PEST to calibrate the one-box NEMURO for the Oyashio region. Climatological monthly data of nitrogen,



**Fig. 4.** RMS of NEMURO model parameters (solid line) and state variables (dotted line) under Exp-4 conditions for different values of the PEST parameters of RELPARMAX and FAXPARMAX, which control the behavior of parameter searching. The RMS values based on parameters compare the values of PEST-estimated parameter values relative to the original (nominal) values. The RMS values based on state variables compare the values of monthly state variables generated using the PEST parameter values relative to the state variables generated with the original values.

silicic acid, total phytoplankton biomass (converted from chlorophyll-*a* concentrations), and zooplankton biomass were determined from available field data. Monthly climatological nutrient and chlorophyll-*a* concentrations were obtained from Ono et al. (2002), and we extended their data from 1999 to 2005. Ono et al. (2002) extracted hydrocast data in the area west of 155°E and north of 36°N in the western North Pacific for 1968–1998 from the JODC database (JODC Data Online Service System; J-DOSS, [http://www.jodc.jhd.go.jp/online\\_hydro.html](http://www.jodc.jhd.go.jp/online_hydro.html)). The database includes data on repeated observation transects, such as the PH-line, A-line, and OICE. Chlorophyll-*a* concentration in  $\mu\text{g L}^{-1}$  was converted to  $\mu\text{mol N L}^{-1}$  by dividing by 1.59 g chlorophyll  $\text{mol N}^{-1}$ . Data for the Oyashio region were selected based on a strict criterion that water temperature was colder than 5 °C at the 100 m depth. Kawai (1972) proposed a slightly different criterion for identifying Oyashio water as less than 33.6 psu and a water temperature colder than a seasonally changing threshold of 5–8 °C at 100 m depth. Sampling stations within 50 km of Japan or the Kuril Islands coast were excluded to avoid the interfusion of Coastal Oyashio Water (melting water from sea ice in the Sea of Okhotsk) with the Oyashio data. Mixed layer depth was defined as a water density change of more than 0.125 from the surface value (Levitus and Boyer, 1994); only data above the computed mixed layer depth were included. All values that satisfied the criteria were identified as Oyashio, and were then averaged for each month of each year for 1968–2005. The averages for each month were then averaged over years to obtain the monthly climatological data.

Monthly zooplankton densities were calculated in a similar manner to chlorophyll-*a*, but using data in the Odate Collection (Odate, 1994; Sugisaki, 2006). Zooplankton density in g-wet-weight  $\text{m}^{-3}$  was converted to  $\mu\text{mol N L}^{-1}$  as follows:

$$\frac{0.2 \text{ g-dry-weight}}{1 \text{ g-wet-weight}} \cdot \frac{0.07 \text{ gN-dry-weight}}{1 \text{ g-dry-weight}} \cdot \frac{1 \text{ molN}}{14 \text{ gN-dryweight}} \cdot \frac{10^6 \mu\text{molN}}{1 \text{ molN}} \cdot \frac{1 \text{ m}^3}{10^3 \text{ L}} = 1 \mu\text{molN} \cdot \text{m}^3 \cdot \text{g-wet-weight}^{-1} \cdot \text{L}^{-1}$$

Values of all the PEST parameters were set to the same values used in the identical twin experiments. Calibration to the normalized field data using PEST involved varying the maximum photosynthesis and zooplankton grazing rates, plus  $R_{\text{SiN}}$ .

Two model simulations were performed: one using the ad hoc determined parameter values reported in Kishi et al. (2007) (labeled “nominal”), and one using the optimal parameter values determined by PEST. The nominal parameter values of NEMURO were developed for Station A7 in the Oyashio region. We compared the nominal and PEST-determined parameter values, and compared the monthly observed data values with the model-simulated values based on the nominal parameter values and on the PEST-determined values.

### 2.5. 3-D-NEMURO simulation of chlorophyll-*a* using calibrated parameters

We ran the 3-D-NEMURO model using the nominal parameter values and the PEST-determined parameter values determined from the calibration to the one-box model using monthly climatological field data. We compared the spatial maps of chlorophyll-*a* for the top 30 m averaged for each of 6 months (January, March, May, July, September, November) for the final year of the simulations. Monthly averaged chlorophyll-*a* concentrations were also obtained from SeaWiFS Level 3 Mapped Monthly Climatology ([ftp://oceans.gsfc.nasa.gov/SeaWiFS/Mapped/Monthly\\_Climatology/CHLO/1997/](ftp://oceans.gsfc.nasa.gov/SeaWiFS/Mapped/Monthly_Climatology/CHLO/1997/)). Thus, three sets of monthly maps were compared: one set based on nominal parameter values, one set based

on the PEST-estimated parameter values from the one-box calibration, and one set from the satellite data.

## 3. Results

### 3.1. Identical twin experiments

PEST was able to accurately recover the original (nominal) parameter values (Table 3) and to closely fit the virtual observations (Fig. 5) in Exp-1. RMS of NEMURO model parameters and state variables were effectively zero. PEST’s success was achieved even though both the phytoplankton and zooplankton information was summed and vertical migration of the large zooplankton was included. The effects of including vertical migration on ZL were seen by the step changes in ZS plus ZL on days 91 and 244 (lower left panel in Fig. 5).

Using slightly different monthly data (averaged instead of snapshots) resulted in PEST-estimated parameter values differing from the original (nominal) values (Exp-2 in Table 3). The largest differences between the monthly snapshots and monthly averages occurred in the spring (days 100–200) because both nutrients and plankton densities were rapidly changing (Fig. 5 versus 6). PEST-estimated parameter values that resulted in close fits of model values to data (Fig. 6), even though these parameter values differed from the original values. The RMS of model parameter estimates was 0.46 and of model state variables was 0.59 in Exp-2. These results demonstrate the possibility of over-fitting and that multiple sets of parameter values can generate similarly good fits to the same data.

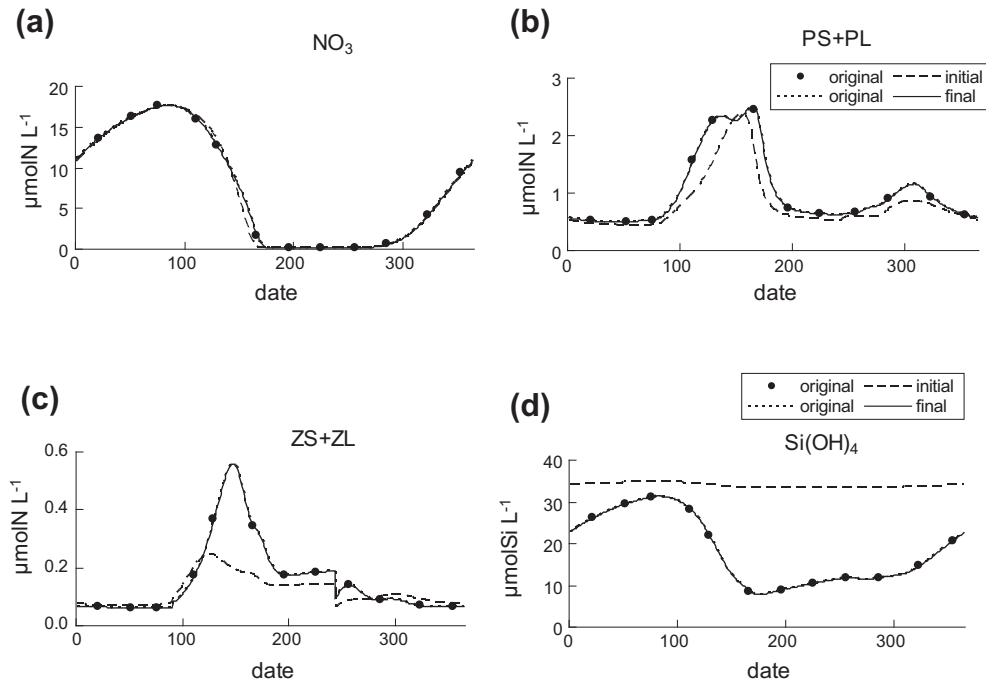
Eliminating vertical migration did not solve the over-fitting problem. PEST successfully recovered the original values with monthly snapshot data without vertical migration (Exp-3 in Table 3), but again not with monthly averaged values even without vertical migration (Exp-4 in Table 3). In both cases without vertical migration, PEST-estimated parameter values resulted in good fits of the model to the data (Figs. 7 and 8). The RMS of model parameters was effectively zero in Exp-3 versus 0.19 in Exp-4, while the RMS of state variables was also zero in Exp-3 versus 0.58 in Exp-4. Vertical migration had some influence, as the PEST-estimated parameter values differed between Exp-2 (including vertical migration) and Exp-4 (excluding vertical migration) (Table 3), both using monthly averaged data. Inclusion of vertical migration increased the RMS of parameter estimation from 0.19 (Exp-4) to 0.46 (Exp-2), while yielding similar fits of the state variables (RMS of 0.58 versus 0.59). The grazing-related parameter values estimated by PEST were similar or higher in Exp-4 than Exp-2, and the value for  $R_{\text{SiN}}$  was higher in Exp-4.

Using the individual functional groups of phytoplankton and zooplankton did not solve the over-fitting problem (Fig. 9). In

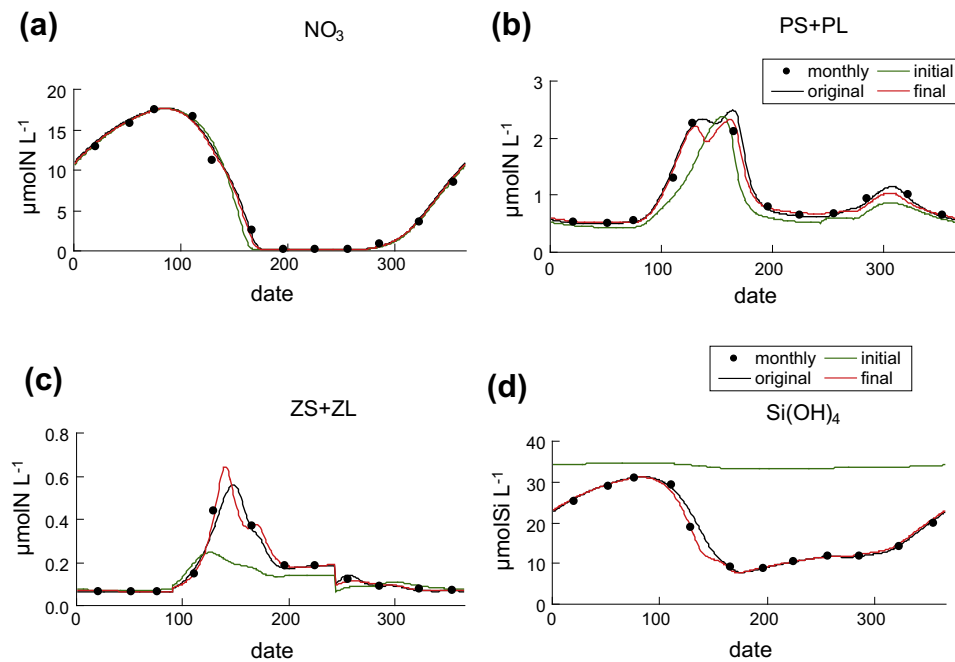
**Table 3**

Original (nominal), initial and PEST-estimated model parameter values in the identical twin experiments.

Parameters	Original values	Initial values	PEST-estimated values				
			Exp-1	Exp-2	Exp-3	Exp-4	Exp-5
$V_{\text{rmaxS}}$	0.40	0.50	0.40	0.38	0.40	0.41	0.42
$V_{\text{rmaxL}}$	0.80	0.50	0.80	0.97	0.80	0.97	0.74
$G_{\text{rmaxZS\_PS}}$	0.40	0.50	0.40	0.19	0.40	0.41	0.45
$G_{\text{rmaxZL\_PS}}$	0.10	0.50	0.10	0.05	0.10	0.11	0.07
$G_{\text{rmaxZL\_PL}}$	0.40	0.50	0.40	0.45	0.40	0.43	0.38
$G_{\text{rmaxZL\_ZS}}$	0.40	0.50	0.40	0.16	0.40	0.66	0.50
$G_{\text{rmaxZP\_PS}}$	0.20	0.50	0.20	0.38	0.20	0.49	0.18
$G_{\text{rmaxZP\_PL}}$	0.20	0.50	0.20	0.15	0.20	0.14	0.23
$G_{\text{rmaxZP\_ZL}}$	0.20	0.50	0.20	0.11	0.20	0.16	0.19
$R_{\text{SiN}}$	2.00	2.00	2.00	3.24	2.00	2.32	2.73



**Fig. 5.** Results of Exp-1. Black dots are the virtual observations, which were monthly snapshots of simulation results (dotted lines, obscured here) calculated by NEMURO with the original (nominal) model parameters. Broken lines are initial solutions of the identical twin experiments which were calculated by NEMURO with the initial parameters. Solid lines are final solutions estimated by PEST.

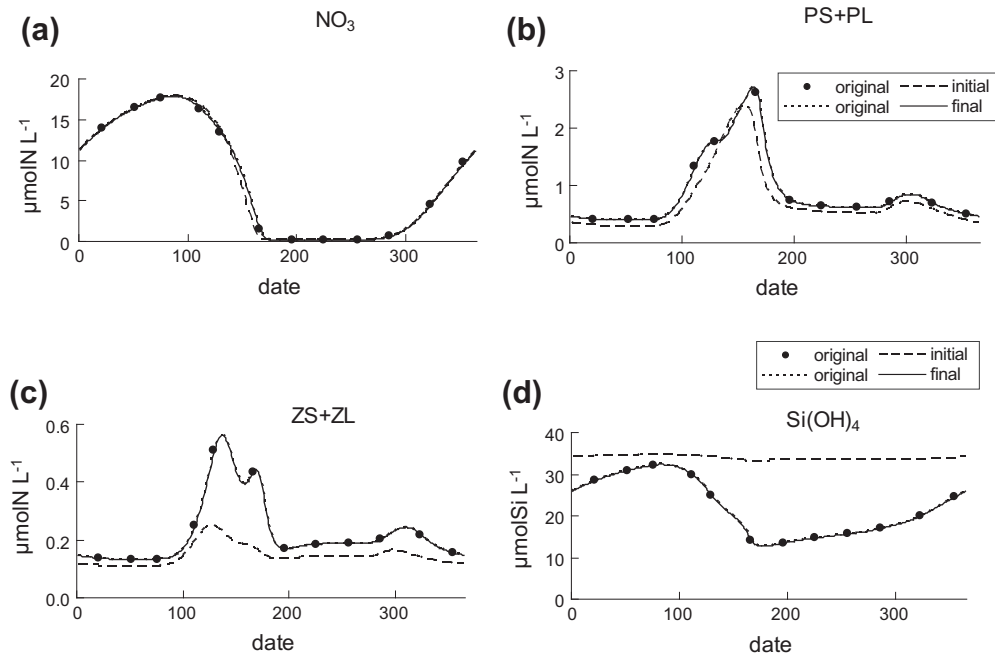


**Fig. 6.** Results of Exp-2. Black dots are the virtual observations, which were monthly snapshots of simulation results (black lines) calculated by NEMURO with the original (nominal) model parameters. Green lines are initial solutions of the identical twin experiments which were calculated by NEMURO with the initial parameters. Red lines are final solutions estimated by PEST.

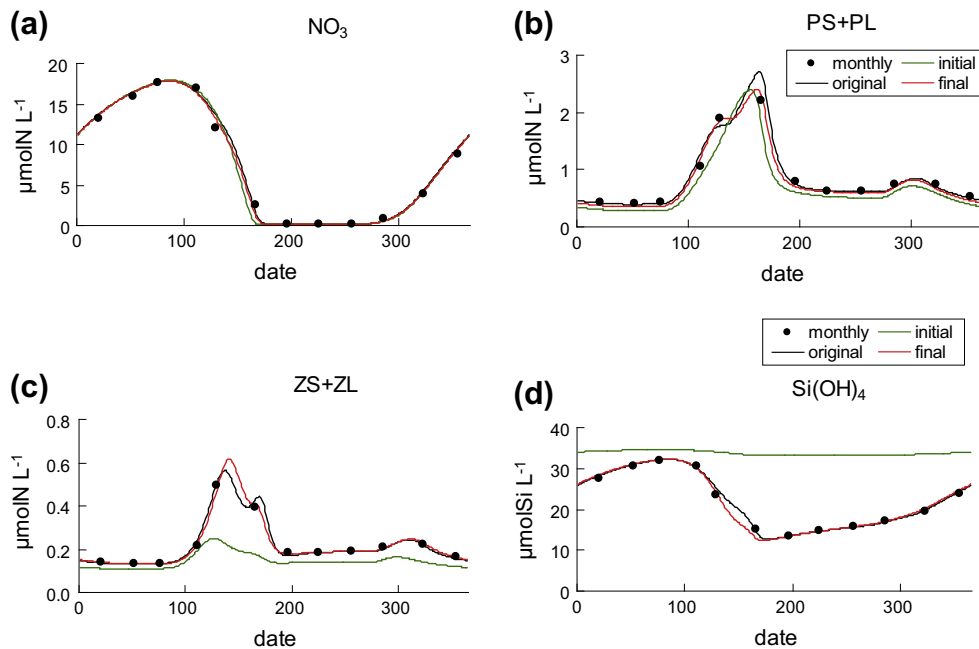
Exp-5, PEST was provided the monthly averaged data of the two phytoplankton groups and the large and small zooplankton groups, without vertical migration, whereas in Exp-4 aggregated values were used. PEST-estimated parameter values in Exp-5 still differed from the original values (Table 3), with some values closer than Exp-4 to the original values and some values further away. For

example, the original value of  $G_{\text{rmaxZP\_PL}}$  was  $0.2 \text{ day}^{-1}$ , and Exp-5 estimated  $0.18 \text{ day}^{-1}$  whereas Exp-4 estimated  $0.49 \text{ day}^{-1}$ . In contrast, the original value of  $R_{\text{SIN}}$  was 2.0, which was more similar to the results of Exp-4 (2.32) than Exp-5 (2.73). RMS values of model parameters were 0.26 in Exp-5 versus 0.19 in Exp-4, while RMS values of state variables were reversed (0.51 versus 0.59).





**Fig. 7.** Results of Exp-3. Black dots are the virtual observations, which were monthly averages of simulation results (dotted lines, obscured here) calculated by NEMURO with the original (nominal) model parameters. Broken lines are initial solutions of the identical twin experiments which were calculated by NEMURO with the initial parameters. Solid lines are final solutions estimated by PEST.



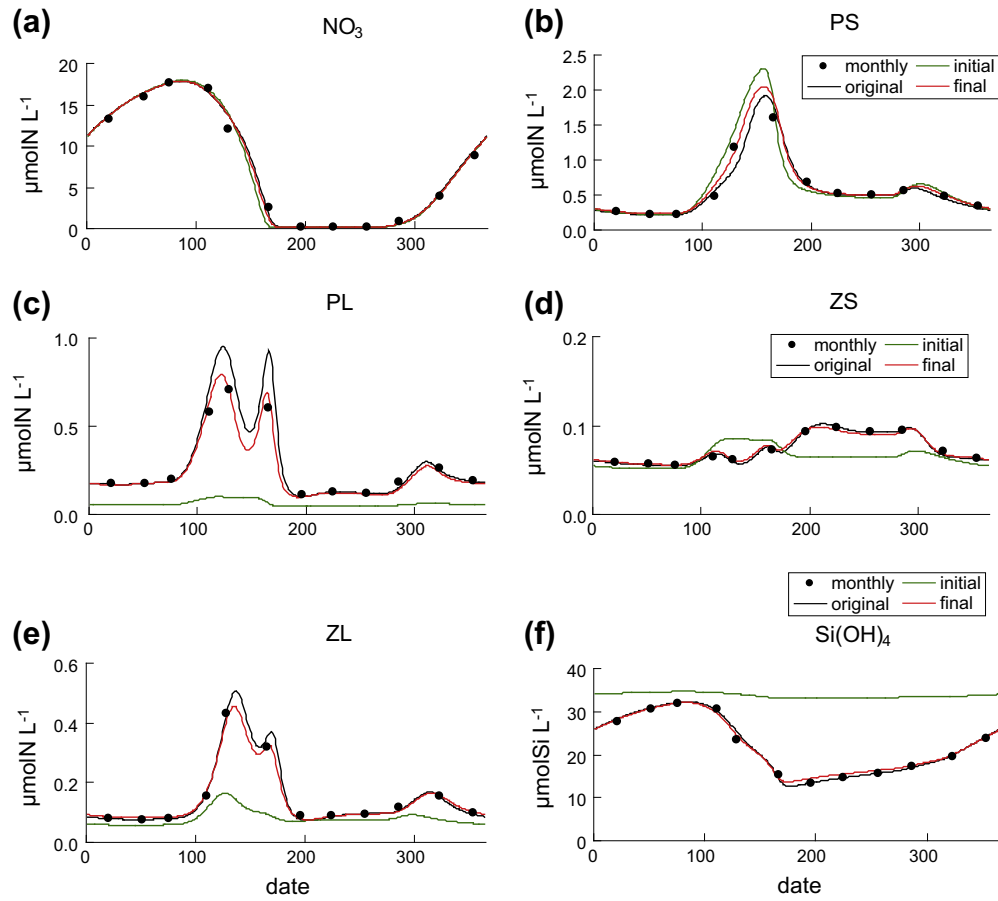
**Fig. 8.** Results of Exp-4. Black dots are the virtual observations, which were monthly averages of simulation results (black lines) calculated by NEMURO with the original (nominal) model parameters. Green lines are initial solutions of the identical twin experiments which were calculated by NEMURO with the initial parameters. Red lines are final solutions estimated by PEST.

### 3.2. Parameter estimation for Oyashio using field data

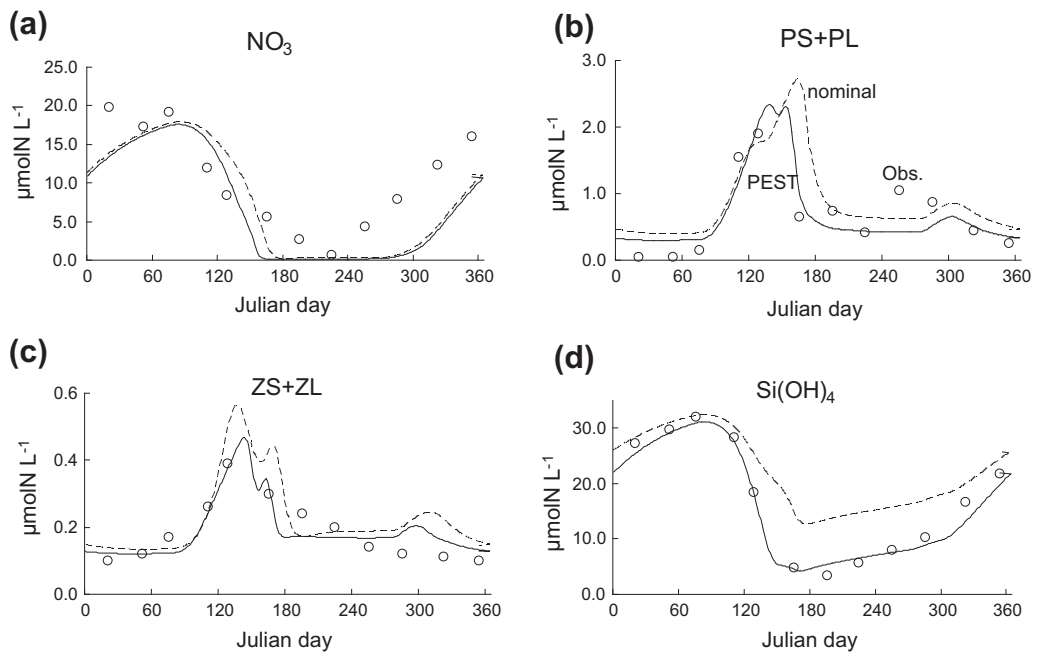
The climatological monthly values based on the field data for the Oyashio showed peak phytoplankton and zooplankton in the spring and minima in nitrate and  $\text{Si(OH)}_4$  in the summer (Fig. 10).  $\text{NO}_3$  and  $\text{Si(OH)}_4$  showed high concentrations from January to March, then decreased from April to August, before recovering from September to December. Total phytoplankton biomass

density (PS plus PL) increased from March to April, showed a maximum in May, and then a second smaller peak in September due to autumn convection (Kishi et al., 2007). The sum of ZS and ZL responded to the phytoplankton spring bloom and also showed a maximum approximately in May.

Simulated values with PEST-estimated parameters were much closer to the field data than with the nominal parameter values (i.e., the ad hoc values reported in Kishi et al., 2007), except for



**Fig. 9.** Results of Exp-5. Black dots are the virtual observations, which were monthly averages of simulation results (black lines) calculated by NEMURO with the original (nominal) model parameters. Green lines are initial solutions of the identical twin experiments which were calculated by NEMURO with the initial parameters. Red lines are final solutions estimated by PEST.



**Fig. 10.** Daily values of model state variables for the Oyashio region simulated using the nominal parameter estimates (dotted line) and parameters estimated by PEST (solid lines). The monthly data are shown as white circles. The nominal parameter values are those reported in Kishi et al. (2007).

**Table 4**

Nominal and PEST-estimated model parameter values when monthly climatological data for the Oyashio region were used as the state variables. The nominal values were those used by Kishi et al. (2007), and were determined by ad hoc calibration.

Parameters	Nominal values	PEST-estimated values
$V_{\max S}$	0.40	0.56
$V_{\max L}$	0.80	1.45
$G_{\max ZS\_PS}$	0.40	0.96
$G_{\max ZL\_PS}$	0.10	0.17
$G_{\max ZL\_PL}$	0.40	0.68
$G_{\max ZL\_ZS}$	0.40	0.66
$G_{\max ZP\_PL}$	0.20	0.70
$G_{\max ZP\_ZS}$	0.20	0.30
$G_{\max ZP\_ZL}$	0.20	0.23
$R_{SiN}$	2.00	1.90

$NO_3$  (labeled “nominal” in Fig. 10). Simulated values with the nominal parameters differed from the field data in several key ways:  $NO_3$  exhaustion from June to September, overestimation of  $Si(OH)_4$  for the summer, peak phytoplankton concentration about 1 month too late, and overestimation of the spring peaks of phytoplankton and zooplankton (Fig. 10). Simulated values with PEST-estimated parameters were closer to the field data and reduced these model-data deviations, except that PEST values also resulted in depletion of  $NO_3$  during the summer. PEST-estimated parameter values generated  $Si(OH)_4$ , summed phytoplankton, and ZS plus ZL concentrations that closely tracked the field data. Diagnostic information generated by PEST during its estimation indicated that the fitting was insensitive to  $NO_3$ . This was likely related to only using a single nitrogen-related variable in the fitting.

PEST-generated parameter values generally resulted in higher phytoplankton production and higher zooplankton grazing rates than the nominal parameter values (Table 4). PEST-estimated values for both maximum photosynthetic rate parameters ( $V_{\max S}$  and

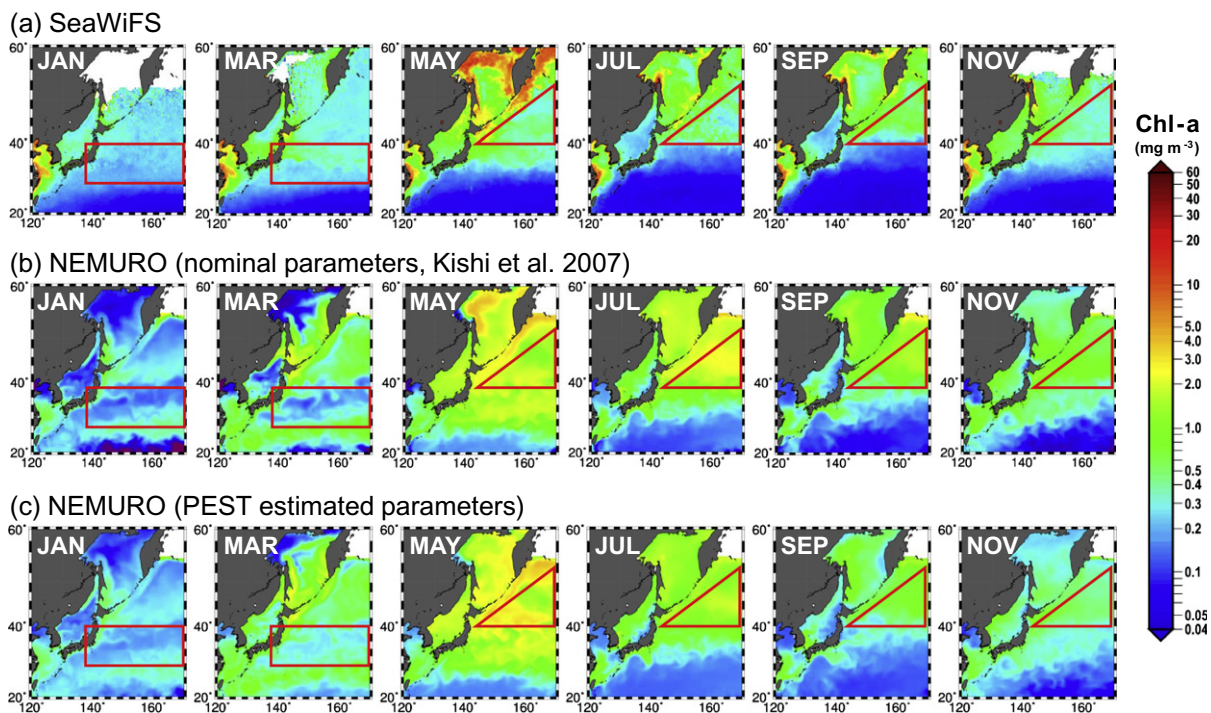
$V_{\max L}$ ) were higher than the nominal values. The largest increases in grazing rate parameters were for  $G_{\max}$  of ZS on PS (0.96 versus  $0.4 \text{ day}^{-1}$ ), ZL on PL ( $0.68$  versus  $0.40 \text{ day}^{-1}$ ), and ZP on PL ( $0.70$  versus  $0.2 \text{ day}^{-1}$ ). The PEST-estimated value for  $R_{SiN}$  changed slightly from the nominal value.

### 3.3. 3-D NEMURO simulation of chlorophyll-*a* maps

Several key spatial features in surface layer chlorophyll-*a* concentration were better simulated using the PEST-estimated parameter values than with the nominal parameter values (Fig. 11). Compared to the satellite-derived values, the nominal parameter values underestimated chlorophyll-*a* concentrations around the Kuroshio Extension during January and March (too much blue), and overestimated chlorophyll-*a* in the subarctic ocean for May to November (too much green and yellow). The PEST-estimated parameter values improved the fit to the satellite data in both cases: simulated chlorophyll-*a* concentrations using the PEST values were higher than those with the nominal parameters in the Kuroshio Extension during January and March (more green, especially in March) and generally lower in the subarctic ocean from May to November (more blue and less green and yellow). PEST-estimated values resulted in additional overestimation of the chlorophyll-*a* concentrations in the subtropical region.

## 4. Discussion

We applied the automated parameter estimation software PEST to estimate optimal parameters for the NEMURO NPZ food web model. Five identical twin experiments were performed. All used monthly values (snapshots or averages) simulated by NEMURO, based on parameter values reported by Kishi et al. (2007), as virtual observations, and involved calibrating two maximum photosynthetic rates, seven zooplankton maximum grazing rates, and



**Fig. 11.** Monthly averaged surface chlorophyll-*a* concentrations. (a) Derived from SeaWiFS satellite data. (b) Calculated by 3-D-NEMURO in the upper 0–30 m layer using nominal model parameters of Kishi et al. (2007). (c) Calculated by 3-D-NEMURO in the upper 0–30 m layer using PEST-estimated parameters. Red outlines show the regions of the Kuroshio Extension and subarctic ocean which are where the PEST-estimated results were closer to the data than the results based on the nominal parameters.

the uptake ratio of silicon to nitrogen by diatoms. PEST started with arbitrary parameter values for the photosynthesis and grazing rate parameters and estimated values that minimized the sum of squared differences between the model-generated monthly values and the virtual data. Ideally, the values of the two photosynthetic rates, seven grazing rates and uptake ratio parameter estimated by PEST would be very similar to the known values that generated the virtual data. The identical twin experiments demonstrated that PEST could recover the known model parameter values, after some adjustment of the PEST parameters that control the search of the NEMURO parameter space. PEST was able to recover the known model parameter values even when non-linear vertical migration of the large zooplankton (ZL) was included. However, when the data were not normalized or when default parameter values of PEST were used, PEST was unable to recover the known NEMURO parameter values. These results demonstrate the importance of data preparation and the details of the fitting procedure when using automatic calibration methods.

Vertical migration of ZL can be problematic for PEST, and likely other automatic calibration methods. In some applications, vertical migration is not needed (e.g., Rose et al., 2007). However, in Kishi et al. (2007) and many other NEMURO related papers, ontogenetic vertical migration of ZL was an important feature of the system. In most of these applications, the vertical migration was defined very simply: all ZL were assumed to migrate out of the modeled box to deeper water layers in autumn and some percent of the diving ZL was assumed to return to the modeled box the next spring. When a single box model is used, this simple vertical migration creates a sharp discontinuity of ZL densities in the modeled box, which can create estimation problems. PEST performed well when vertical migration was included in our analyses, but required some adjustments in how PEST searched the NEMURO parameter space; initially, default values of PEST parameters were unable to recover the known NEMURO parameter values. Vertical migration may be less of a problem in a vertically-resolved model because the deep ZL are still part of the model output and PEST and other calibration methods may be able to better deal with their movements with proper definition of state variables and calibration parameters. NEMURO has been imbedded in 1-D vertical physical models for several locations (e.g., Fujii et al., 2002; Smith et al., 2005).

A new complication with vertically-resolved versions of NEMURO will be that the model state variables become spatially-explicit (i.e., depth profiles over time). This requires many more data for calibration, although PEST has been used previously for parameter estimation involving dynamic spatially-explicit state variables and parameters (e.g., Bravo et al., 2002; Lin and Radcliffe, 2006). Another possibility that would take account of ZL densities year round is a simple 2-box model configuration (explicit representation of the deep box) in which PEST could be provided with state variables for each box or summed for the water column (e.g., Terui and Kishi, 2008). We have also not exhausted all possible ways to adjust PEST for vertical migration in NEMURO-based models. Some other possibilities include adding state variables to account for ZL when it is deep, ignoring zero ZL densities, performing the parameter estimation in multiple steps, and including the NEMURO migration parameters as parameters to be estimated by PEST. Also, the PEST software is continuing to be refined and developed (e.g., Skahill et al., 2009). At this point, we recommend that PEST be used with caution in applications that involve discontinuous functions, such as the vertical migration function used here. Appropriate parameter values can be estimated but care must be taken in how the data are prepared and the values used for the searching parameters of PEST.

Our results clearly show the potential for parameter over-fitting and the importance of data preparation. What appeared to be slight differences in the monthly data provided to PEST (snapshots

versus averages), resulted in similar fits to the data but with very different values for the NEMURO parameters. Exp-1 was able to recover the original values, whereas Exp-2 was unsuccessful; similarly, Exp-3 recovered the original values but Exp-4 did not. Exp-1 and Exp-2 both included vertical migration but Exp-1 used snapshot values whereas Exp-2 used averaged values. Exp-3 and Exp-4 both did not include vertical migration and also only differed by whether snapshot or averaged data were used. This tendency for over-fitting is partly because of exhaustive searching by PEST, especially with the non-default values of NPHINORED, RELPARMAX and FACPARMAX, which were needed for successful parameter estimation with vertical migration but allowed for continued evaluation of parameter searching beyond default values. But it can also lead to over-tuning of the NEMURO model parameters. This over-fitting problem was not solved by increasing the resolution of the data (i.e., using each functional group separately). Including vertical migration may have worsened the over-fitting problem. The RMS of estimated NEMURO parameter values was 0.46 in Exp-2 versus 0.19 in Exp-4, suggesting the estimated model parameters were further from the original values in Exp-2 than in Exp-4. Therefore, careful preparation of the data and application of PEST, and other calibration methods, is needed for these methods to be reliable with NEMURO-like NPZ models.

We applied PEST to the real field data for the Oyashio, and compared model fits and parameter values to those from Kishi et al.'s (2007) calibration to Station A7. We eliminated the vertical migration of large zooplankton, but still used the Kishi et al. (2007) parameter values that were initially determined with vertical migration included. PEST was able to estimate parameter values that resulted in reasonably good fits to the monthly field data. These fits were an improvement over those obtained using the Kishi et al. (2007) parameter values, except for the depletion of  $\text{NO}_3$  in the summer that was predicted with both the PEST-estimated parameters values and the Kishi et al. (2007) parameter values. The parameter values estimated by PEST were consistently larger than those of Kishi et al. (2007), implying that with the PEST values, primary production and predation rates were faster and hence energy flow was enhanced in the system. When these same two sets of parameter values were substituted into 3-D-NEMURO (without vertical migration), the PEST-estimated parameter values generated spatial maps that were more similar to the satellite data in several ways than those generated with the Kishi et al. (2007) parameters. Simulated chlorophyll-*a* concentration using the PEST-estimated values were more similar to the data for the Kuroshio Extension during January and March and in the subarctic ocean from May to November.

PEST estimated higher values of  $V_{\max}$  and  $Gr_{\max}$  for the Oyashio compared to those used by Kishi et al. (2007) for Station A7. The Kishi et al. (2007) values ( $0.4 \text{ day}^{-1}$  for PS and  $0.8 \text{ day}^{-1}$  for PL) were based on Eppley (1972). Recently, phytoplankton data were collected for the Oyashio. The dominant taxa during the spring bloom were *Thalassiosira*, *Chaetoceros*, and *Fragilariopsis* species, and their  $V_{\max}$  value was estimated in laboratory experiments as  $0.6 \text{ day}^{-1}$  with a 14-h light and 10-h dark condition (Kuwata, 2009). Therefore, under 24-h light conditions,  $V_{\max}$  can be estimated as  $1.24 \text{ day}^{-1}$ . This estimate, based on site-specific information, was higher than the value used by Kishi et al. (2007) ( $0.8 \text{ day}^{-1}$ ), which lends partial support to the higher values estimated by PEST ( $1.45 \text{ day}^{-1}$ ). Only limited site-specific information is available for the  $V_{\max}$  of PS.

Estimates of zooplankton maximum grazing rate parameters are also limited, but some site-specific information is available. Kobari et al. (2008) estimated copepod community ingestion rates in the surface (0–150 m) as  $213\text{--}375 \text{ mgC m}^{-2} \text{ day}^{-1}$  and determined that this accounted for 26 to 37% of primary production. The biomass of copepods was between 1732.9 and 3370.6  $\text{mgC m}^{-2}$ . We can use this information to derive a rough estimate of  $Gr_{\max}$ . Using



the higher ingestion rate estimate, the ratio of ingestion to biomass was  $0.111\text{--}0.125\text{ day}^{-1}$ . We converted this to a maximum rate at  $0\text{ }^{\circ}\text{C}$  under unlimited prey. Sea surface temperature during the data collection varied from  $9.6\text{ }^{\circ}\text{C}$  to  $11.1\text{ }^{\circ}\text{C}$ ; we used  $10\text{ }^{\circ}\text{C}$ , which, with the Q10 value, leads to multiplying by 0.5 to get the rate expected at  $0\text{ }^{\circ}\text{C}$ . To adjust for prey limitation, we used the climatological data from the Oyashio region (i.e., prey concentration of  $2.0\text{ }\mu\text{mol N L}^{-1}$ , Fig. 10) and, using the Kishi et al. (2007) parameter values for the Ivlev function, computed a prey limitation effect of 0.244. Adjusting the field estimates for temperature and prey limitation results in an estimated value of  $Gr_{\text{max}}$  of  $0.23\text{--}0.26\text{ day}^{-1}$ . The PEST-estimated values were generally similar to, or higher than this site-specific estimate (Table 4), suggesting that the parameter values estimated by PEST may be too high. More site-specific information is needed to determine the realism of the PEST-estimated maximum grazing rate parameters.

The version of NEMURO used in this analysis ignores possible iron limitation and uses mortality closure terms for zooplankton, which can create confounding problems for parameter estimation. Our version of NEMURO used here does not take into account the effects of micro-nutrients such as iron, which is potentially important in the North Pacific (e.g., Tsuda et al., 2003; Moore et al., 2004; Yoshie et al., 2005). Iron limitation is presently being added to NEMURO. If iron limitation was important in the modeled region, PEST would try to adjust the other parameters to account for the missing iron limitation effects, resulting in biased parameter values.

Similarly, predation on the zooplankton by fish, cephalopods, and marine mammals are represented by a simple mortality rate based on the squared zooplankton biomass. Other versions of NEMURO include fish predation of zooplankton explicitly and have shown that the predation rates can vary in time and space (e.g., Megrey et al., 2007; Ito et al., 2004c). In addition, for the Oyashio, the very high biomass of Japanese sardine in the 1980s had a large effect on zooplankton (Tadokoro et al., 2005; Ito et al., 2007), which would affect field observations of zooplankton densities. As with ignoring iron limitation, the over-simplified representation of predation mortality in NEMURO will force PEST to adjust other parameters in order to match the field data. These problems are common to many NPZ models because all models must simplify some aspects of the system. Minimization of these confounding effects requires careful use of automatic calibration software and use of available field and laboratory data to constrain model parameters.

Our analysis here for the Oyashio was similar to the analysis by Rose et al. (2007) for the West Coast Vancouver Island location in the eastern North Pacific. Both analyses applied one-box versions of NEMURO to roughly monthly climatological field data and compared parameter values based on ad hoc calibration with those estimated by PEST. In Rose et al. (2007), the PEST-estimated value for  $V_{\text{max}}$  was slightly higher than the ad hoc value for PS (0.56 versus 0.49) and much lower for PL (0.25 versus 0.71). In this study, the PEST value was also higher than the ad hoc value for PS (0.56 versus 0.4) but much higher for PL (1.45 versus 0.8). This suggests that PEST may have difficulty in parameter estimation for models that cover spatial areas or domains that include sub-regions with different characteristics, similar to other optimization methods. Ultimately, incorporating automatic calibration directly into a broad-domain model like 3-D-NEMURO will need to deal with how to optimize multiple parameter sets distributed among sub-regions.

We recommend using PEST, or other parameter optimization methods, for estimating parameter values of NPZ models. The first step would be to develop a climatological dataset, and use PEST to generate first-order parameter estimates. Sensitivity analysis (*sensu* Yoshie et al., 2007) could be used to identify the subset of parameters needing accurate estimation, which should then be adjusted in the automatic calibration. As much as possible, auxiliary

laboratory and field data should be used to constrain model parameter values. Various configurations of the state variables should also be investigated to determine the robustness of the parameter estimates. Identical twin experiments, which are relatively easy to implement, provide confirmation that model parameters are estimable. If a reasonable set of parameter values can be determined when applied to the field data, they provide an excellent starting point for other model analyses, such as 3-D implementations. Parameter estimates should be viewed cautiously because of estimation issues related to migration of biota in and out of the modeled box, sensitivity of the estimates to how the data were summarized, and confounding effects that arise from simplifications (e.g., ignoring iron limitation; mortality closure terms; simplified physics) in the NPZ model. Confirming the method with identical twin experiments and comparing parameter values based on ad hoc calibration with automatic calibration provides valuable information on model behavior and performance. The inconsistencies between simulated values and the available field data provide valuable information on the dynamics of the ecosystem.

### Acknowledgements

We wish to acknowledge GLOBEC and PICES for supporting the development of the NEMURO family of models. Especially, members of PICES CCCC MODEL task team contributed to model developments. We also wish to thank the captain and crew of Hokko-maru, Wakataka-maru, Kofu-maru and other observation ships and scientists on those ships who maintain repeated observations in the Oyashio region. We thank M. Friedrichs and anonymous reviewers for their invaluable suggestions. This work was done under the Global Warming Project supported by Ministry of Agriculture, Forestry, and Fisheries Japan. The participation of BAM in this paper is noted as research contribution EcoFOCI-0730 to NOAA's Ecosystem and Fisheries-Oceanography Coordinated Investigations. Bernard A. Megrey died on 1 October 2010 while this paper was being prepared. He was a collaborator and a friend, and he will be missed.

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