Adjoint Assimilation of SeaWiFS data into a Marine Ecosystem Dynamical Model of the Bohai Sea and the North Yellow Sea

C. H. Wang, X. Y. Li, X. Q. Lv*

Laboratory of Physical Oceanography, Ocean University of China, Qingdao, 266100, China

Abstract

A three-dimensional coupled physical-biological model involving variational adjoint assimilation was applied to the Bohai Sea and the North Yellow Sea (BNYS), utilizing real chlorophyll data from the Sea-Viewing Wide Field-of-view Sensor (SeaWiFS). The coupled model consists of a simple three-dimensional Nutrient-Phytoplankton-Zooplankton-Detritus (NPZD) model and a primitive-equation physical model. There are 12 ecological parameters in the NPZD model. All these parameters are assumed to be time-varying. By using the data assimilation technique, the optimal values of these parameter were estimated, and the seasonal variabilities of these parameters were reconstructed. We find that some parameters are highly correlated, and they may have some internal relations. The time variances of most parameters seem reasonable. And the annual cycles of the estimated parameters may help us to improve the performance of the model. The comparison between simulation and observation shows that after assimilation of SeaWiFS data the output of the NPZD model agrees better with the observation.

Keywords: ecosystem modeling; variational adjoint assimilation; SeaWiFS; Bohai Sea and North Yellow Sea

1. Introduction

In the past few decades, people pay more and more attention to the global climate change, how to improve numerical modeling ability on climate change has become significantly important. Marine dynamical ecosystem models with various levels of sophistication have been developed for different

*Corresponding author. Tel.: +86-0532-66782971; fax: +86-0532-82032471
E-mail address: xqinglv@ouc.edu.cn.
regions of the ocean. The dimension of the models ranges from zero-dimension [1,2], vertical one-dimension [3,4] and horizontal two-dimension [5,6] to three-dimension [7-11]. The number of biological parameters and state variables are significantly different. For example, there are 4 state variables and 12 ecological parameters in Qi’s [12] model but 11 and 75 correspondences in the North Pacific marine ecosystem(NEMURO [13]). The simulating time of the models were also different, varies from 8 days [14] to one year [15].

It seems that in the past almost all the researchers assumed the ecological parameters to be constants which did not change with time and space in their studies. But in reality, the ecological parameters are influenced by physical environment and biological composition. Errors generated from constant parameters in the study area can not decrease effectively by adding new ecological mechanisms or improving physical background, so some researchers began to use spatially varying ecological parameters in the past decade. In Losa’s [16] work, a simple NPZD model was coupled to a 3-dimensional general circulation model (POP), which underestimated both the average chlorophyll level and its regional variability from middle to high latitudes with constant biological model parameters over the whole basin. Experiments with either a different parameterization of heat and freshwater fluxes or advection of the biological tracers turned off made a negligible impact on phytoplankton patterns. Only model run with spatially varying biological parameters, obtained from Losa’s [17] zero-dimensional ecosystem model calibration on CZCS ocean colour data, could reproduce regional scale patterns in the SeaWiFS imagery. Fan’s [11] results also show that spatially variable parameters are more reasonable than a set of constants. The errors are much smaller, and regional features in the SeaWiFS imagery can be reproduced much better.

Unfortunately, hardly any of the researchers assumed the model parameters to be changed with time before. So in this paper, we treat the ecological parameters as temporal-dependent variables to improve the performance of ocean ecosystem model, and the variational adjoint technique is used to assimilate the SeaWiFS chlorophyll data into the ecological model and to estimate the annual cycle of the optimal parameters values. The paper is organized in the following manner. Section 2 describes the model and the adjoint method. Results and discussion are given in Section 3. The conclusions of our work are presented in Section 4.

Fig. 1. Water depth of the Bohai Sea and the Yellow Sea (m).
2. Model

The simulation area includes the Bohai Sea and the North Yellow Sea (BNYS) (34.5°-41°N, 117.5°-127.5°E). The open boundary is at 34.5°N. Figure 1 shows the topography of the BNYS.

2.1. The physical model

The three-dimensional Princeton Ocean Model (POM) is used to calculate the ambient physical velocities, the temperature, and the eddy diffusivities. The model is forced at the open boundary by both the climatological circulation and the surface tides, including four tidal components (M₂, S₂, K₁ and O₁). The monthly mean temperature and salinity are taken from Levitus data, and wind speed data come from SOC (Southampton Oceanography Center).

2.2. The biogeochemical model

Based on the Nutrient-Phytoplankton-Zooplankton (NPZ) model of Franks [18], detritus is added as a state variable to construct a three-dimensional ecosystem model in the BNYS. This type of model which is also termed NPZD model is widely used to simulate the marine ecosystem [19-22].

The NPZD model here (Fig.2) includes the primary biological and chemical processes, for example, the photosynthesis of phytoplankton, the grazing of phytoplankton by zooplankton, the assimilation of ingested phytoplankton by zooplankton, the excretion of zooplankton, the death of phytoplankton and zooplankton, the regeneration of detritus, and so on. In the model, nitrogen is used as a tracer for the state variables. Dissolved nutrients are taken up by the phytoplankton following Michaelis-Menten kinetics, while phytoplankton is grazed by zooplankton with an Ivlev functional response. The impacts of temperature on the phytoplankton and zooplankton growth are described by Q₁₀ rule [23]. The nutrients which input into the BNYS from rivers, the air, and the sediment are considered.

![Diagram of the NPZD model](image-url)

Fig. 2. Diagram of the NPZD model.
The primitive equations of the NPZD model are described in Appendix A. The initial values of ecological parameters taken from previous researchers [5,23-25] are summarized in Table 1.

Table 1. Ecological parameters and their initial values

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Initial value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_m$</td>
<td>phytoplankton maximum photosynthetic rate at 10°C</td>
<td>1.8</td>
<td>/day</td>
</tr>
<tr>
<td>$G_m$</td>
<td>zooplankton maximum grazing rate at 10°C</td>
<td>0.5</td>
<td>/day</td>
</tr>
<tr>
<td>$d_p$</td>
<td>phytoplankton mortality rate</td>
<td>0.1</td>
<td>/day</td>
</tr>
<tr>
<td>$d_z$</td>
<td>zooplankton mortality rate</td>
<td>0.1</td>
<td>/day</td>
</tr>
<tr>
<td>$e$</td>
<td>remineralization rate of detritus</td>
<td>0.0212</td>
<td>/day</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>zooplankton Ivlev constant</td>
<td>0.2</td>
<td>m$^3$/mmol N</td>
</tr>
<tr>
<td>$k_{ext}$</td>
<td>light extinction coefficient</td>
<td>0.1</td>
<td>/m</td>
</tr>
<tr>
<td>$AQ_{10}$</td>
<td>phytoplankton temperature coefficient for growth</td>
<td>2.08</td>
<td>/</td>
</tr>
<tr>
<td>$BQ_{10}$</td>
<td>zooplankton temperature coefficient for growth</td>
<td>3.1</td>
<td>/</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>zooplankton growth efficiency</td>
<td>0.3</td>
<td>/</td>
</tr>
<tr>
<td>$\theta$</td>
<td>zooplankton excretion rate</td>
<td>0.4</td>
<td>/</td>
</tr>
<tr>
<td>$k_s$</td>
<td>half-saturation for nitrogen uptake</td>
<td>1.0</td>
<td>mmol N/m$^3$</td>
</tr>
</tbody>
</table>

The biological model is discretized on the Arakawa-C grid. The horizontal resolution is $10' \times 10'$ ($1/6^\circ \times 1/6^\circ$), and the Cartesian coordinate in the vertical is used. There are 6 vertical layers in the biological model. The vertical grid sizes are 10m, 10m, 10m, 20m, 25m and 25m. To study the temporal variations of ecological parameters, we split one year (360 days) into 72 parts on temporal average. Each part is an independent sub-model with the same set of initial parameter values but different initial conditions. The time steps of the NPZD model and the adjoint model are both 30 minutes.

2.3. Initial and boundary conditions

The initial value of the chlorophyll concentration is the multi-year averaged historical statistic observation. Since only sea surface chlorophyll concentration can be recovered, statistic method is used to get the empirical vertical structure of chlorophyll concentration. We collect the chlorophyll data at 44 stations in the simulated area and calculate the ratio of chlorophyll concentration of each layer to that of the surface layer. The result is shown in Fig. 3. Chlorophyll concentration in each layer can be obtained by interpolating sea surface chlorophyll data linearly according to the vertical distribution in Fig. 3(b).
The external sources of nutrient include the major river loads and the atmospheric wet and dry deposition. The fluxes of nutrient from land and atmosphere are obtained from the literatures [26,27] and linearly interpolated to each time step. The zero-gradient condition is used for the state variables.

2.4. Observation

In the present study, surface chlorophyll data representative of the phytoplankton are assimilated into the NPZD model. And these data are derived from Sea-Viewing Wide Field-of-view Sensor (SeaWiFS) monthly averaged ocean color data in 2003 and are linearly interpolated into each time step. The ratio of N:Chl for phytoplankton is 605mmol N(g Chl-a)^{-1}.

2.5. Adjoint method

One problem of applying the ecosystem models to reality is that a large number of parameters are poorly known, such as phytoplankton maximum photosynthetic rate. It is difficult to determine the parameter values by measurement because of the lack of observations. And we can not directly apply the values measured in laboratory experiments to a real system, because the environment conditions are much more complicated and changing all the time. Data assimilation techniques are vital tools to find the optimal parameter values objectively by contrasting the discrepancy between the model outputs and the observations. One of the generally used assimilation method in physical-biological coupled models is the variational adjoint method. Many researchers applied adjoint technique to getting the optimum parameter values to improve the accuracy of the ecosystem models [1, 4, 28-35].

Adjoint assimilation can automatically minimize the misfit between the simulation results and the corresponding observations by modifying the control variables including initial conditions, boundary conditions and model parameters. The cost function which is usually used to measure the misfit, is defined as:

\[ J = \frac{1}{2} \sum_{i,n} (x_{i,n} - \bar{x}_{i,n})^2 \]  

where x and \( \bar{x} \) are the model outputs and the observations, respectively, \( i \) refers to the available observation types and \( n \) refers to the observation time. \( W_i \) are the weights of the observations, and it takes into account the relative magnitude of the various data types and the quality of the data sets [31]. In this paper, only SeaWiFS chlorophyll data are assimilated, so \( W_i \) are defined as:

\[ W_i = \begin{cases} 
1, & \text{if } \bar{x}_{i,n} \text{ exists} \\
0, & \text{otherwise} 
\end{cases} \]  

By introducing Lagrange multipliers, the adjoint model can be constructed. The adjoint model provides a method of calculating the gradient of the cost function with respect to the control variables. The gradient is used to determine the direction to change the vector of control variables. A new estimation of the control variables can be obtained by using the value of the cost function and the value of its gradient, and this process continues iteratively until the control variables converge to the values that minimize the cost function or a preset convergence criterion is satisfied, e.g. \( J \leq \varepsilon^1 \) or/and \( \| \nabla J \| \leq \varepsilon^2 \), where \( \| \nabla J \| \) is the norm of the gradient of the cost function, and \( \varepsilon \) denotes a small value. The values of the control variables which give the minimum of the cost function can be considered as the optimal ones. More details can be found in Lawson [1,28] and Zhao [14]. The workflow to apply adjoint assimilation...
method into ecosystem is shown in Fig. 2 [31,34-36], the adjoint equations and formulas used to calculate the gradients of the cost function are shown in appendix B and C, respectively.

Fig. 4. The workflow of the adjoint assimilation: The solid lines indicate the main path taken during the procedure.
Fig. 5. Model-produced co-tidal charts for M2, S2, K1 and O1 tides (a, b, c and d, respectively): solid lines are phase-lag (deg) and dashed lines are amplitude (cm).
3. Results and discussions

3.1. Co-tidal charts

The model-produced co-tidal charts are shown in Fig. 5. The co-tidal charts of the semidiurnal constituent $M_2$ and $S_2$ are similar. There are four amphidromic points in the simulated area, which are located in the Liaodong Bay, the Huanghe estuary, the sea area near Chengshantou and the southern waters of Shandong Peninsula. There is only one amphidromic point of diurnal constituent in the computational domain, and it is located in the Bohai Strait. It seems that there is another amphidromic point in the center of South Yellow Sea, just outside the computational domain. The results are consistent with those of Fang [37], Guo [38] and Lefevre [39].

3.2. Cost function

As shown in Fig. 6, the cost function descends significantly, indicating the simulated results are more consistent with the observations after assimilation. The minimum value of the cost function before assimilation is about $1 \times 10^5$. After assimilation, all the cost functions in the year descend, and the maximum value of the cost function is less than $7.5 \times 10^4$. The ratio of final cost function to its initial value is smaller than 50 percent at most time of a year, meaning that the assimilation method is effective for all the cycles.
Fig. 6. The cost function versus time in a year: (a) the initial cost function when first-guess values of the control variables are given; (b) the final cost function after the optimal values of control variables are obtained; (c) the ratio of final cost function to its initial value.

![Cost Function Graph](image)

Fig. 7. Ratio of cost function to its initial value versus assimilation step.

Fig. 7 shows the ratio of cost function to its initial value versus assimilation steps. The ratio is averaged over the 72 cycles. It is clear that the cost function descends rapidly at first twenty assimilation steps, and then it reaches a steady state, indicating that the variation of the parameters influences the model outputs a little. So we can say that the adjoint technique is computationally efficient to recover the optimal model parameters.

The simulated annual cycle of chlorophyll in BYNS is shown in Fig. 8. The model result using the first-guess values of the parameters compares poorly with the observation. The simulated chlorophyll concentration is much larger than the observation in all parts of the year. And a phytoplankton bloom occurs in early July in the model result, but it doesn’t occur in the observation. After assimilation, the result agrees much better with the observation, indicating that the adjoint technique improve model output effectively. But the simulated chlorophyll concentration is a little smaller than the observation, and this may be caused by the misfit between the model structure and the observation.

![Chlorophyll Concentration Graph](image)

Fig. 8. Simulated and observed chlorophyll concentration in BNYS (mg/m^3). Dashed line denotes result using first-guess values of the parameters, solid line denotes result using optimal values and solid line with fork denotes observation from SeaWiFS in 2003.
3.3. Model parameters

3.3.1. Correlations of parameters

The optimal values of the 12 parameters during a year can be obtained from the output of the adjoint model, and they are shown in Fig. 9(a)-(f). The correlation coefficients between any two parameters are shown in Table 2.

From Fig. 9 and Table 2 we can see that there is certain correlativity between the 12 parameters. Take Fig. 9(a) for example, it is clear that $G_m$ and $\gamma$ are highly positively correlated, and the correlation coefficient is 0.829. With the increase of $G_m$, more phytoplankton grazed by zooplankton is assimilated.

For Fig. 9(b), the correlation coefficient between $k_{ext}$ and $d_p$ is 0.701. Generally the death of phytoplankton is in direct proportion to the living biomass. If the phytoplankton biomass increases, the death rate increases accordingly. At the same time, the increase of phytoplankton will reduce the transparence of sea water, meaning that the light extinction coefficient $k_{ext}$ is increased. Besides, both McGillicuddy [30] and Radach [40] expressed the light extinction coefficient $k_{ext}$ as a function of chlorophyll concentration, and it increases with the increase of chlorophyll concentration. This shows that $k_{ext}$ is also in direct proportion to phytoplankton biomass. Thus we can draw the conclusion that the phytoplankton death rate $d_p$ is in positive correlation with the light extinction coefficient $k_{ext}$. Fig. 9(b) obviously shows us this positive correlation.

Table 2. Correlation coefficient between model parameters

<table>
<thead>
<tr>
<th></th>
<th>$G_m$</th>
<th>$d_p$</th>
<th>$d_z$</th>
<th>$e$</th>
<th>$\lambda$</th>
<th>$k_{ext}$</th>
<th>$AQ_{10}$</th>
<th>$BQ_{10}$</th>
<th>$\gamma$</th>
<th>$\theta$</th>
<th>$k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_m$</td>
<td>-0.110</td>
<td>0.352</td>
<td>-0.481</td>
<td>-0.529</td>
<td>0.412</td>
<td>0.125</td>
<td>0.456</td>
<td>-0.384</td>
<td>-0.208</td>
<td>-0.185</td>
<td>0.615</td>
</tr>
<tr>
<td>$G_m$</td>
<td>0.596</td>
<td>0.005</td>
<td>-0.168</td>
<td>0.639</td>
<td>0.558</td>
<td>0.565</td>
<td>-0.584</td>
<td>0.829</td>
<td>-0.499</td>
<td>0.066</td>
<td></td>
</tr>
<tr>
<td>$d_p$</td>
<td>-0.565</td>
<td>-0.569</td>
<td>0.762</td>
<td>0.701</td>
<td>0.787</td>
<td>-0.704</td>
<td>0.478</td>
<td>-0.175</td>
<td>0.484</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.3.2 Time variations of parameters

As shown in Fig. 9, the optimized model parameters change significantly with time. Some of the changes do make sense. For example, the microbiology points out that the maximum growth rate occurs when the population density is optimum [41]. Once the population density is larger than the optimum density, the growth rate will reduce because of the limited nutrient and environment conditions. And the optimization result of $V_m$ implies that there is a connection between the growth rate and the phytoplankton concentration which are not included in this ecological model. A similar example is $G_m$. Many biological experiments indicate that if the density of prey is changeless, the interference between the individuals induces the grazing rate to reduce with the increase of the density of predator. As shown in Fig. 10, the annual variation of $G_m$ increases with the reduction of the zooplankton concentration, revealing the relation between the grazing rate and the predator density. In our model, the death term of the zooplankton is expressed as a linear process of zooplankton concentration. But it is also usually modeled as a nonlinear process [9], which implies the death rate is density-dependent—higher death rate at higher zooplankton density. From the result of the time variation of $d_z$, we can find that $d_z$ and the zooplankton concentration are positively correlated, indicating a nonlinear expression of death term is more feasible in our model. So the annual cycles of the parameters may help us to improve the model, but there is still a lot of work need to do to explain the meaning of the time variations of the rest parameters.

<table>
<thead>
<tr>
<th>Variable</th>
<th>d_0</th>
<th>e</th>
<th>$\lambda$</th>
<th>$k_{ext}$</th>
<th>$AQ_{\theta}$</th>
<th>$BQ_{\theta}$</th>
<th>$\gamma$</th>
<th>$\theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.718</td>
<td>-0.613</td>
<td>-0.579</td>
<td>-0.553</td>
<td>0.539</td>
<td>-0.218</td>
<td>-0.093</td>
<td>-0.783</td>
</tr>
<tr>
<td></td>
<td>-0.971</td>
<td>-0.298</td>
<td>-0.694</td>
<td>0.724</td>
<td>-0.270</td>
<td>0.436</td>
<td>-0.794</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.784</td>
<td>0.811</td>
<td>-0.772</td>
<td>0.643</td>
<td>-0.440</td>
<td>0.679</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.622</td>
<td>-0.548</td>
<td>0.616</td>
<td>-0.016</td>
<td>0.423</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.844</td>
<td>0.521</td>
<td>-0.391</td>
<td>0.467</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.547</td>
<td>0.372</td>
<td>-0.569</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.428</td>
<td>0.166</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.01</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 10. Seasonal variability of zooplankton, $G_m$ and $d_z$. 
4. Conclusion

In the traditional numerical simulation, the estimation of model parameters depends on the experiences and iterative debugging, and there is always too much work to do for a satisfying result. Although some investigators have applied the adjoint technique to parameter estimation in recent studies [1, 4, 10-12, 28-35], almost all of them treated the ecological parameters as constants in their studies. Only a few of them [11,12] assumed the ecological parameters to be spatially varied but none treated the parameters as time varying variables. In this study, all the biological parameters are assumed to be time varying. By assimilating the SeaWiFS chlorophyll data, we reconstruct the seasonal variability of the 12 optimized ecosystem model parameters. The result shows that the variety tendencies of some parameters are the same or reverse, indicating that they may have some internal relations. After assimilation, the cost function decreases to 25% of its initial value on average, and the simulated results using optimal parameter values accord much better with the observations.

The optimized results of $V_m$, $G_m$ and $dZ$ are reasonable. The time variations of the parameters can reveal the potential relation between the parameters and the state variables, and it is helps to improve the biological model. But more work need to be done to reveal the meanings of the time variations of other parameters.

The chlorophyll data from SeaWiFS is larger than the cruise data in the Bohai Sea in the entire year, especially in winter. The observed chlorophyll concentration increases from the southeast to the northwest, and its minimum(2.5 mg/m$^3$) is in the southeast of the Central Bohai Sea and its maximum concentration is about 4.0 mg/m$^3$. The observed chlorophyll concentration in the Bohai Sea is very small because the shallow depth of the Bohai Sea and the strong wind in winter intensify the mixing of the sea water. The detritus formed by death phytoplankton is returned to the sea surface by mixing, and the sensor in the satellite misjudge the part of detritus to living chlorophyll, causing overvalue of the chlorophyll concentration. So the chlorophyll data of the Bohai Sea from SeaWiFS is not appropriate to be assimilated into the model, and the optimum parameter values in winter need further study.

These are just preliminary results of adjoint assimilation applied to marine dynamical ecosystem models. The model will be improved in the later study, and more observations are needed to be assimilated.

Acknowledgements

The authors acknowledge the support of the State Ministry of Science and Technology of China under contract NO.2007AA09Z118 and NO.2008AA09A402, the National Natural Science Foundation of China through grant 41076006 and the Ministry of Education’s 111 Project through grant B07036.

References


Appendix A. Primitive equations

\[
\frac{\partial P}{\partial t} + u \frac{\partial P}{\partial x} + v \frac{\partial P}{\partial y} + w \frac{\partial P}{\partial z} = \frac{\partial}{\partial x} (A_n \frac{\partial P}{\partial x}) + \frac{\partial}{\partial y} (A_n \frac{\partial P}{\partial y}) + \frac{\partial}{\partial z} (K_n \frac{\partial P}{\partial z}) 
+ \frac{V_N}{k_p + N} \cdot e^{-k_p z} \cdot A_{Q_{10}}^{(7-10)/10} \cdot P - G_n \cdot B_{Q_{10}}^{(7-10)/10} \cdot (1 - e^{-\lambda P}) \cdot Z - d_n P
\]

(3)

\[
\frac{\partial Z}{\partial t} + u \frac{\partial Z}{\partial x} + v \frac{\partial Z}{\partial y} + w \frac{\partial Z}{\partial z} = \frac{\partial}{\partial x} (A_n \frac{\partial Z}{\partial x}) + \frac{\partial}{\partial y} (A_n \frac{\partial Z}{\partial y}) + \frac{\partial}{\partial z} (K_n \frac{\partial Z}{\partial z}) 
+ \gamma G_n \cdot B_{Q_{10}}^{(7-10)/10} \cdot (1 - e^{-\lambda P}) \cdot Z - d_z Z
\]

(4)
\[
\frac{\partial N}{\partial t} + u \frac{\partial N}{\partial x} + v \frac{\partial N}{\partial y} + w \frac{\partial N}{\partial z} = \frac{\partial}{\partial x} \left( A_{\text{H}} \frac{\partial N}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_{\text{H}} \frac{\partial N}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{\text{H}} \frac{\partial N}{\partial z} \right) \\
- \frac{V N}{k_{\text{H}} + N} \cdot e^{-s_{\text{K}}} \cdot A_{Q_{\text{H}}}^{(T-10^{10})/10} P + \theta \cdot G_{w} \cdot BQ_{\text{H}}^{(T-10^{10})/10} \cdot (1 - e^{-\lambda P}) \cdot Z + eD
\]

(5)

\[
\frac{\partial D}{\partial t} + u \frac{\partial D}{\partial x} + v \frac{\partial D}{\partial y} + w \frac{\partial D}{\partial z} = \frac{\partial}{\partial x} \left( A_{\text{H}} \frac{\partial D}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_{\text{H}} \frac{\partial D}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{\text{H}} \frac{\partial D}{\partial z} \right) \\
+ (1 - \gamma - \theta)G_{w} \cdot BQ_{\text{H}}^{(T-10^{10})/10} \cdot (1 - e^{-\lambda P}) \cdot Z + d_{w} P + d_{z} Z - eD
\]

(6)

where \( P \) is the phytoplankton, \( Z \) is the zooplankton, \( N \) is the dissolved nutrient and \( D \) is the detritus, all of their units are converted into \( \text{mmolN} \cdot \text{m}^{-3} \). The ambient physical velocities are \( u, v \) and \( w \), while the horizontal and vertical eddy diffusivities are \( A_{\text{H}} \) and \( K_{\text{H}} \), respectively. The phytoplankton sinks with speed \( w_{s} \), and \( T \) is the temperature of seawater.

Appendix B. Ajoint Equations

\[
- \frac{\partial P'}{\partial t} - \frac{\partial}{\partial z} \left( K_{\text{H}} \frac{\partial P'}{\partial z} \right) = \frac{\partial}{\partial x} \left( uP' \right) + \frac{\partial}{\partial y} \left( vP' \right) + \frac{\partial}{\partial z} \left( wP' \right) + w_{s} \frac{\partial P'}{\partial z} \\
+ \frac{\partial}{\partial x} \left( A_{\text{H}} \frac{\partial P'}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_{\text{H}} \frac{\partial P'}{\partial y} \right) \\
+ \frac{V N}{k_{\text{H}} + N} \cdot e^{-s_{\text{K}}} \cdot A_{Q_{\text{H}}}^{(T-10^{10})/10} \left( P' - N' \right) - d_{w} \cdot (P' - D')
\]

(7)

\[
\frac{\partial Z'}{\partial t} - \frac{\partial}{\partial z} \left( K_{\text{H}} \frac{\partial Z'}{\partial z} \right) = \frac{\partial}{\partial x} \left( uZ' \right) + \frac{\partial}{\partial y} \left( vZ' \right) + \frac{\partial}{\partial z} \left( wZ' \right) \\
+ \frac{\partial}{\partial x} \left( A_{\text{H}} \frac{\partial Z'}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_{\text{H}} \frac{\partial Z'}{\partial y} \right) \\
- G_{w} \cdot BQ_{\text{H}}^{(T-10^{10})/10} \left( 1 - e^{-\lambda P} \right) \left( P' - \gamma \cdot Z' - \theta \cdot N' - (1 - \gamma - \theta) \cdot D' \right)
\]

(8)

\[- d_{z} \cdot (Z' - D')\]
\[
- \frac{\partial N^*}{\partial t} - \frac{\partial}{\partial z} \left( K_n \frac{\partial N^*}{\partial z} \right) = \frac{\partial}{\partial x} (uN^*) + \frac{\partial}{\partial y} (vN^*) + \frac{\partial}{\partial z} (wN^*) \\
+ \frac{\partial}{\partial x} (A_{n} \frac{\partial N^*}{\partial x}) + \frac{\partial}{\partial y} (A_{n} \frac{\partial N^*}{\partial y}) \\
+ \frac{V_n k_i}{(k_s + N)^2} \cdot e^{-k_s z} \cdot AQ_{10}^{(7-10)/10} \cdot P \cdot (P' - N') \\
\]

\[
- \frac{\partial D^*}{\partial t} - \frac{\partial}{\partial z} \left( K_n \frac{\partial D^*}{\partial z} \right) = \frac{\partial}{\partial x} (uD^*) + \frac{\partial}{\partial y} (vD^*) + \frac{\partial}{\partial z} (wD^*) \\
+ \frac{\partial}{\partial x} (A_{n} \frac{\partial D^*}{\partial x}) + \frac{\partial}{\partial y} (A_{n} \frac{\partial D^*}{\partial y}) \\
+ e \cdot (N' - D') \\
\] (9)

where \(N^*, P^*, Z^*\) and \(D^*\) are the adjoint variables corresponding to \(N, P, Z\) and \(D\) respectively in the adjoint equation.

**Appendix C. The Gradients of the Cost Function**

\[
\frac{\partial J}{\partial N_n} = -\frac{N}{k_s + N} \cdot e^{-k_s z} \cdot AQ_{10}^{(7-10)/10} \cdot P \cdot (P' - N') \\
\] (11)

\[
\frac{\partial J}{\partial k_s} = \frac{V_n N}{(k_s + N)^2} \cdot e^{-k_s z} \cdot AQ_{10}^{(7-10)/10} \cdot P \cdot (P' - N') \\
\] (12)

\[
\frac{\partial J}{\partial G_n} = BQ_{10}^{(7-10)/10} \cdot (1 - e^{-\lambda}) \cdot Z \cdot Temp \\
\] (13)

\[
\frac{\partial J}{\partial \lambda} = G_n \cdot BQ_{10}^{(7-10)/10} \cdot e^{-\lambda} \cdot P \cdot Z \cdot Temp \\
\] (14)

\[
\frac{\partial J}{\partial \theta} = -G_n \cdot BQ_{10}^{(7-10)/10} \cdot (1 - e^{-\lambda}) \cdot Z \cdot (N' - D') \\
\] (15)

\[
\frac{\partial J}{\partial \gamma} = -G_n \cdot BQ_{10}^{(7-10)/10} \cdot (1 - e^{-\lambda}) \cdot Z \cdot (Z' - D') \\
\] (16)

\[
\frac{\partial J}{\partial k_{ext}} = \frac{V_n N}{k_s + N} \cdot e^{-k_s z} \cdot z \cdot AQ_{10}^{(7-10)/10} \cdot P \cdot (P' - N') \\
\] (17)

\[
\frac{\partial J}{\partial AQ_{10}} = -\frac{V_n N}{k_s + N} \cdot e^{-k_s z} \cdot \frac{T - 10}{10} \cdot AQ_{10}^{(7-10)/10} \cdot P \cdot (P' - N') \\
\] (18)

\[
\frac{\partial J}{\partial \theta} = G_n \cdot \frac{T - 10}{10} \cdot BQ_{10}^{(7-20)/10} \cdot Z \cdot (1 - e^{-\lambda}) \cdot Temp \\
\] (19)
\[
\frac{\partial J}{\partial d_p} = P \cdot (P' - D') \\
\frac{\partial J}{\partial d_z} = Z \cdot (Z' - D') \\
\frac{\partial J}{\partial e} = -D \cdot (N' - D') \\
\text{Temp} = P' - \gamma Z' - \theta N' - (1 - \gamma - \theta)D'
\]