Integration of ocean-colour remote sensing with coastal nowcast/forecast simulations of harmful algal blooms


19.1 Introduction

Forecasting harmful algal blooms is one example of the larger effort to predict community phytoplankton populations in the marine environments. Early modelling efforts attempted to mathematically solve for the growth and loss of phytoplankton (also known in today’s literature as sources and sinks) in a fairly straightforward method (see Mills, 1989; Riley, 1946):

\[
\frac{dP}{dt} = P(P_h - R - G)
\]  

(19.1)

where the time-dependent change in phytoplankton populations \( P \) is equal to the initial phytoplankton population multiplied by the net of the terms for the phytoplankton specific growth rate \( P_h \), minus respiration \( R \) and grazing rate \( G \). This equation is the basis of all phytoplankton models and 60 years after its authorship is still used with minor modifications (c.f. McGillicuddy et al., 2006 – Chapter 16 this volume).

Equation (19.1) illustrates the basic concept in ocean ecological modelling. This concept simply states the concentration of a phytoplankton at a given point in time is dependent on its growth rate, its respiration rate and its loss (grazing) rate. The application of this conceptual model becomes more complicated in practice. The concentration of phytoplankton at a given point in time and space is a function of a fully three-dimensional environment where phytoplankton cells may move via sinking or swimming, while also being moved by the circulation of water (Franks, 2006 – Chapter 15 this volume). In addition, the movement of the phytoplankton coupled with the movement of water alters the light and nutrient niches in which the phytoplankton are living, thereby providing ecological feedbacks that impact the net accumulation of phytoplankton biomass (Bissett et al., 2001). While (19.1) offers the foundation, the nuances as to how and why specific phytoplankton taxa accumulate are more complicated and require a more thorough description. For over 100 years, researchers have attempted to acquire this greater ecological knowledge of phytoplankton processes by conducting both laboratory and field experiments. These experiments have led to better quantification of the factors controlling the light and nutrient assimilation dynamics of phytoplankton, and in turn have led to more complex parameterization of (19.1) (e.g. Andersen and Nival, 1988; Anderson, 1993; Anderson and Williams, 1998,
Habwatch


The increase in complexity was, in part, to help describe the ever-expanding relationships being described in the observational community. The complexity was also embraced because of an increasing amount of research that found improved stability with increasing complexity, i.e. increasing species, diversity, functional groups and interaction strength (the likelihood that one species will consume another) (Fussmann and Heber, 2002; McCann and Hastings, 1998; Naeem and Li, 1997; Naeem et al., 1994; Tilman et al., 2001). This helped to overcome some of the problems associated with numerical instabilities in simple ecological models (May, 1973a).

HAB forecasting is especially difficult since one is trying to predict the ecology of a single phytoplankton population within a much larger community of phytoplankton species (estimated to number over 30,000: Falkowski and Raven, 1997). The traditional nutrient-phytoplankton-zooplankton (NPZ) model (or its extension nutrient-phytoplankton-zooplankton-detritus, NPZD) focused on population assemblages as a whole, using the N term as the model currency, and converting phytoplankton biomass into an easily measured proxy for biomass, i.e. chlorophyll, for validation. This approach is useful for describing general ocean systems, but HAB forecasting requires an understanding and quantification of the competitive interactions within phytoplankton populations, such that a single phytoplankton taxa may be quantitatively described. Thus, the numerical model that one selects for the purpose of predicting a HAB must have the flexibility to effect differential growth and loss rates across many simulated phytoplankton species, so that under the ‘right’ environmental conditions the HAB population is adequately simulated (e.g. Yamamoto et al., 2002).

Over the last few years, optics has found a place at the intersection of numerical phytoplankton studies and HAB research. Ocean optics offers a means to sample both the bulk properties of the water column over large temporal and spatial ranges, as well as the individual properties of phytoplankton populations down to the cell (see Chang and Dickey, 2006; Lewis, 2006; Morel, 2006; Sosik, 2006; Babin, 2006; Schofield et al., 2006 – Chapters 2, 6, 4, 8, 7 and 3 this volume). It also offers the ability to quantify a niche dimension for phytoplankton simulations by virtue of describing the intensity and colour of the ambient light field as one moves deeper in the water column. This numerical description of changing spectral quality and magnitude provides an optical niche dimension by which phytoplankton may differentiate themselves against competitors in different environments depending on the optically active constituents in the water.
example, if there are large concentrations of optical constituents, i.e. phytoplankton and coloured degradational matter (CDM), typical of eutrophic coastal environments, the photon density will decrease very rapidly with depth and will transition from green to yellow in its spectral distribution. In the Sargasso Sea, where the water is oligotrophic with little phytoplankton biomass or CDM, the photon density decreases more slowly with depth and becomes blue-green in spectral distribution. The resulting light field (and nutrient regime) will select for those phytoplankton that can best use the resources, i.e. in the deep Sargasso Sea one may find small Prochlorococcus spp. rich in chlorophyll \( b \) that are ideally suited to absorb the low photon densities of blue-green light. Simulating the time-dependent change in the ambient light field along with the time-dependent change of optical constituent concentrations provide a quantifiable means of imparting feedback mechanisms into numerical simulations (Bissett et al., 2001), which can be validated from aircraft and space-based remote sensing, as well as with \textit{in situ} measurements (e.g. Bissett et al., 1999a). Thus, by integrating the prediction of optics into nowcast/forecast systems that seek to predict HABs, HAB forecasting may be directly merged with remote sensing HAB identification techniques (e.g. Stumpf et al., 2003).

The simulation of water column optical properties requires additional complexity in the formulation of an ecological model’s structure and parameterization. The model must specifically address and quantify those properties that do not change with respect to the geometry of the light field, the inherent optical properties (IOPs), and those that are dependent on the directionality of the photon density, the apparent optical properties (AOPs, see Morel, 2006 – Chapter 4 this volume). IOPs, such as absorption and scattering, are directly related to individual phytoplankton taxa, as well as to other optical constituents, such as CDM and sediments. AOPs, which include remote sensing reflectance \( R_{rs} \), and the diffuse attenuation coefficient \( K_d \), are dependent on the IOPs and the radiance distribution (i.e. geometry) of the downwelling light field. Since the IOPs and the AOPs are interrelated, sampling the AOPs from space or aircraft allows for the estimation of IOPs via empirical or analytical inversion techniques. From the estimation of IOPs, one may estimate the various properties of the phytoplankton assemblage, such as total pigment (e.g. Gordon et al., 1983) and/or carbon biomass and productivity (e.g. Behrenfeld et al., 2005), through empirical or analytical algorithms that relate reflected ocean colour to the phytoplankton properties. It may also be possible to use the spectral characteristics of phytoplankton specific IOPs, which are directly related to phytoplankton taxa, and thereby separate the bulk property signals into specific taxa stocks (Kirkpatrick et al., 2000; Millie et al., 1995; Millie et al., 1997; Roesler et al., 2003). All these optical inversion techniques are part of active research programmes, and as such are not without errors. The successful application of these optical techniques would provide critical HAB stock assessment for model initialization, as well as model validation, which might then allow for the ability to assimilate and predict the occurrence of HABs within a nowcast/forecast system.\(^9\)

The use of a simplified approach to the parameterizing of the terms of (19.1) may be constructive in qualitatively describing the interaction of light and nutrients in aquatic systems. The use of optics as a means to provide additional niche spaces by

\(^9\) It should be explicitly acknowledged that this application of coupling optics to HAB population density would most probably apply to those HAB populations that produce a high enough optical signal to be remotely sensed. An example of these populations would include those on the West Florida shelf (Stumpf et al., 2003). However, in areas where the HAB density is too low to alter the optical signal from the background noise, this hypothesized approach would not be (as) successful. An example of this type of HAB would include \textit{Alexandrium} in the Gulf of Maine (Cullen, 2006 – Chapter 1 this volume).
which to effect phytoplankton competition, as well as provide additional mechanisms to initialize and validate HAB forecasts, requires an increase in the complexity of the nowcast/forecast system beyond those earlier modeling efforts. In deriving new models to predict specific HABs, one must find balance between the requirements for quantitative prediction and qualitative understanding in constructing the numerical model format, where quantitative results such as cell numbers of harmful phytoplankton taxa or physical units of $R(\lambda)$ may be separated from less robust measures of phytoplankton biomass, i.e. chlorophyll. In this balancing process, one may find it impossible and/or unnecessary to simulate the entire suite of phytoplankton in a particular region in order to generate a reasonable forecast of local HABs. For example, one may reduce the full assemblage of phytoplankton to a representative few functional groups with similar optical, nutrient uptake, and allometric characteristics (e.g. Bissett et al., 1994, 1999b) in order to address the ecological question at hand. Since there has been (at the date of this report) no generalized solution for phytoplankton or HAB prediction, the degree of model complexity will be user, problem and site specific. In the model-selection process, care must be taken to avoid numerical transient problems (e.g. limit cycles) associated with numerical models (e.g. May, 1971, 1973a, 1973b), which are often driven by simplified equations and unrealistic physical conditions used to describe complex environmental and ecological interactions. Thus, it is important in the model construction process to match complexity and structure to the scientific question being asked, thereby arriving at an 'appropriate' model formulation. An appropriate model is defined here as one that can address the ecological question at hand, whose parameters are as constrained as possible from field and laboratory data, thereby limiting parameter tuning to a minimum. In addition, an appropriate model would offer the potential for quantitative prediction and validation.

The component most frequently unconstrained in (19.1) is the loss or grazing term $G$. This term is frequently the 'closure' term of phytoplankton numerical models (see Steele and Henderson, 1992). The closure term is the parameter, which when tuned is likely to cause the generation of simulation results that are the most acceptable during the model evaluation process. The loss term is frequently based on estimates of grazer populations, viral and bacterial phages and/or mass dependent sinking fluxes as a function of phytoplankton biomass concentration. The weak constraint on this component is in part a result of the difficulties in sampling grazer populations and their clearance rates, as well as other relatively undefined loss processes, such as mass dependent viral and bacterial phage transmission, and/or apoptosis. When the model structure for (19.1) is expanded to explicitly include herbivore zooplankton, this closure problem is expanded to include those difficulties surrounding higher trophic levels and may cause a geometric expansion of the unconstrained parameters. In contrast to the loss processes, the phytoplankton nutrient uptake rates, assimilation rates, pigment concentrations, and growth rates are more easily measured in the laboratory. Thus, there are often detailed formulations of the growth component of (19.1), while the loss component is more often parameterized with a more simplified equation that may be easily modified as a function of temperature and seasonality. Unfortunately, any closure method is fraught with validation difficulties, and what may be a reasonable simulation in one time/space location, may yield very spurious results in another location.

As mentioned above, the circulation of the water plays an important role in the production and accumulation of any phytoplankton population, including HABs. In

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91 Given the diversity of HABs, there may never be a 'generalized' numerical solution (Cullen, Chapter 1).
numerical simulations, this is frequently the largest source of error in the validation of numerical predictions and forecasts. Some ecological simulation techniques are more sensitive than others but all require that the advection and diffusion equations place the right parcel of water in the right place at the right time. Without adequately resolving the physics, it is very difficult to generate realistic simulations of HABs; and while it may be possible to numerically simulate a HAB, the likelihood of it being a valid forecast is often limited because the simulated environmental conditions did not match the actual environmental conditions. Forecasting a tornado in a sun shower is not a realistic result and woe betide the modeller who attempts to explain the errors in a HAB simulation as the result of growth and loss dynamics, when the real culprit may be a poorly constrained physical model. However, a perfect physical model does not currently exist and the exploration of ecological dynamics should proceed even in light of the imperfections in the physical modelling effort. In some cases, the errors in the physical model may not create a qualitative, or even drastic quantitative, error in the overall ecological solution. In evaluating the ecological result, one must attempt to separate the physical errors from the biological, optical, and chemical ones, in order to achieve some level of system understanding into causal ecological dynamics.92

In order to demonstrate a representative ecological and optical simulation of phytoplankton populations, including the HAB species *Karenia brevis* (*K. brevis*), the results of the phytoplankton dynamics of a numerical study of the West Florida Shelf (WFS) will be described. It is based on a two-dimensional simulation used to predict IOPs and CDM distributions on the WFS during summer/autumn 1998 (a complete description of the model may be found in Bissett et al., 2005). In the precursory study by Bissett et al., it was determined that the addition of a terrestrial boundary condition was required to reasonably simulate the IOPs and CDM distributions over this period. To be shown here are the impacts of these terrestrial boundary conditions, rich in colour and nutrients, on the phytoplankton functional groups, including *K. brevis*, as well as the impacts on the water-leaving radiance signal that may be seen by satellite. In addition, a sensitivity study to the closure term in the model will demonstrate the impact of this parameter on the individual phytoplankton functional groups, as well as the bulk optical properties and remote sensing reflectance.

Our goal is to describe a set of ecological and biogeochemical interaction equations that allow for the differentiation and competition of algal classes based on temperature, light and nutrients. This model is derived for the coastal zone and as such includes terrestrial boundary conditions in a consistent manner that preserves its numerical stability while providing results that are directly comparable to the available validation data streams. The work described here goes hand in hand with a previous paper that describes a set of ecological interaction equations incorporating optics as a fundamental component of its structure (Bissett et al., 2005). The focus of this modelling effort is to specifically avoid reductionism, which would provide only a minimal set of interaction equations that describes this specific site and data set. The goal of this larger effort is to apply a broad set of ecological equations to multiple environments with minimal parameter tuning, such that its application may be robust across

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92 While some may read this as an indictment of the physical model, such is not the case. It is meant solely to recognize that the formulation and validation of ecological models, which are critically dependent on the physical circulation models, need to progress along with the physical model development. The ecological models tend to be far less developed for a wide variety of reasons, not least of which is that there are no ‘fundamental’ ecological equations similar to the hydrostatic approximation equations with which to build the ecological formulations and structure.
multiple ecotones (transitional zones between two communities containing the characteristic species of each). This approach would allow for a single ecological model to be used for multiple coastal regimes within the same simulation experiment.

19.2 Methods

The model used here tracks the time-dependent change of 89 state variables which include seven functional groups of phytoplankton, two classes of dissolved organic matter, two classes of faecal material, one heterotrophic class of bacteria (as well as an inferred nitrification class of bacteria), and six inorganic nutrient stocks, including carbon, nitrate, ammonium, silica, phosphorus and iron (Bissett et al., 2005). It is a coastal expansion of an open ocean simulation, which separated carbon and nitrogen dynamics to more accurately account for carbon cycling in the Sargasso Sea (Bissett et al., 1999a, 1999b). The model uses non-stoichiometric nutrient uptake, assimilation and regeneration, which allows for niche separation based on nutrient type and quantity. The photosynthetic properties of the phytoplankton functional groups are described with individual pigment suites, which are allowed to vary as a function of light and nutrient history. This allows for niche separation as a function of spectral photon density. All optically active constituents are described with absorption and scattering equations to drive a spectral light model that attenuates light with depth at 5 nm spectral resolution. The physics is supplied by a two-dimensional spatial (offshore and depth) circulation model driven by winds and boundary conditions on the WFS during 1998. The resulting depth-dependent IOPs are supplied to a fast radiative transfer model, Ecolight, which is a derivative of the Hydrolight model to yield the prediction of water-leaving radiance. The simulation was run for three numerical years with the exact same forcing to reduce numerical transient responses to the boundary conditions, such that year-over-year changes in the stocks were less than 0.5%. The full numerical description of the model may be found in Bissett et al. (2005).

19.2.1 Shoreward boundary conditions

The shoreward and offshore boundary conditions were unchanged from those previously described by Bissett et al. (2004, 2005). Nutrient data for the Charlotte Harbor region was collected from seven sources. These nutrients constituted the shoreward boundary condition. Organic nitrogen was found to be a major contributor to total nitrogen concentrations in this region and inorganic phosphorus was also a key nutrient due to the proximity of this location to the Hawthorne Phosphatic Formation. Discharges from the local rivers (the Peace River and the Caloosahatchee River) coincided with peaks in nutrient concentrations in 1998 (Figure 19.1). The shoreward boundary conditions were simulated by an increase in nutrients and total colour concentrations at the shoreward boundary model cell reproducing a riverine flux for day-of-year (DOY) 267 (24 September) and 309 (5 November). This is possibly a conservative estimate of the ecologically significant mass additions to the shelf during these periods, as the outflow events driving the decreases in salinity would have occurred over the course of several days (or possibly weeks). An accompanying freshwater flux and change in buoyancy was not simulated due to the two-dimensional nature of this model, and the physical constraints made it impractical to hydrologically model the freshwater mass. It is clear that the baroclinic flows would be altered by these events; however,
it is beyond the scope of this effort to predict those impacts. The gulf-side boundary conditions changed seasonally and were derived from the 1998/1999 ECOHAB cruises on the WFS (Figure A.1, Bissett et al., 2005).

19.2.2 Optical model

Light harvesting by phytoplankton is assumed to be a function of the available downwelling energy at depth and the absorption spectra of each phytoplankton functional group. The absorption spectra of each functional group are not static, but rather are dependent on the light and nutrient history of each functional group at each grid point. This allows for the differentiation of phytoplankton by pigment suites and spectral photosynthetic efficiencies, providing competitive advantages to those species that can optimize light absorption and photochemical conversion at different depths and colour zones. In this model, an explicitly defined suite of IOPs was developed for each optical constituent in the model, i.e. phytoplankton, CDOM, detritus, etc. Time-dependent changes in these mass constituents drove the associated modifications in the coupled IOPs. The IOPs were then used to calculate.

Figure 19.1
Total daily discharge from the Peace River measured at the USGS station ‘Peace River at Arcadia’ (red line) displaying elevated discharges in early and late 1998 with corresponding elevated concentrations of total nitrogen (TN) measured at the USGS station ‘Peace River at River Mile 3.95’ near Punta Gorda, Florida (black circles) along with total daily discharge from the Caloosahatchee River at the Franklin Lock and Dam (S79) (blue line).
the Apparent Optical Properties (AOPs) of downwelling irradiance, \( E(\lambda) \), with a numerically efficient single scattering approximation (Bissett et al., 1999a). This allows us to validate the biogeochemical simulation with in situ IOP and AOP instruments, as well as spectral remote sensing products from multispectral or hyperspectral satellite and aerial sensors when these simulated IOPs are used in conjunction with a robust radiative transfer model, i.e. Hydrolight (see Bissett et al., 2005, for a full description).

19.2.3 SeaWiFS processing and analysis

SeaWiFS processing and analysis was previously described by Bissett et al. (2005). Raw SeaWiFS processing was performed at the Naval Research Laboratory Stennis, Mississippi, by the Ocean Sciences Branch, Code 7330. This processing included an iterative atmospheric correction scheme that reduced the errors found in the standard SeaDAS processing for near-shore coastal waters. The region of interest on the WFS originated at the 10 m isobath and extended approximately 60 km offshore. Since the offshore islands of the region were shoreward of the 10 m isobath, they were not accounted for in this simulation. The boundary of the region was designated by the coordinates \([27.2957N, 83.3415W], (27.5396N, 82.7993W), (26.2062N, 82.7200W), (26.4502N, 82.1830W)\] (Bissett et al., 2005, Figure A.1). Lines of data were resampled at 30 equally spaced intervals between these points using the SeaWiFS Data Analysis System (SeaDAS) and then splined to 1 km increments perpendicular to the coast. This was required to normalize the data pixelization that occurs as a function of SeaWiFS scan angle and SeaDAS projection angle relative to the coast of the WFS. The mean of these 30 lines (numbered from Tampa Bay south to Charlotte Harbor) and the mean plus and minus one standard deviation were then plotted. The mean of lines 22–30 (near Charlotte Harbor) were also plotted since this location is the focus of the study.

19.2.4 Ecolight

The radiative transfer solution to produce simulated remote sensing reflectance \(R_s\) at the surface of the water was given by a model derived from Hydrolight. Ecolight reduces the computation requirement of Hydrolight in two major ways. The first is by band averaging over azimuthal angles, eliminating the azimuthal dependence terms of the radiative transfer equation (RTE), and eliminating the Fourier decomposition of the radiance or the RTE. The second is an estimate of the maximum relevant depth to the radiometric quantity of interest and is made prior to the calculation of the RTE. This allows for the selection of an optical depth for which to solve, and an estimate of the geometric depth with which to solve to. These simplifications allow the full RTE to be calculated for upwelling light based on the simulated IOPs in a computationally efficient manner, i.e. Ecolight is orders of magnitude faster than Hydrolight, without loss of accuracy in the upwelling and downwelling estimates of photon densities.93 This allows for the direct validation of predicted photon densities to remote sensing data.

The greatest benefit of ecological modelling is that the upwelling light field contains all the optical information on the vertical structure of the IOPs. Accurate simulation

93 There are ways to optimize Ecolight for more speed, but such further optimization results in loss of accuracy.
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of remote sensing reflectance would suggest validation of the vertical structure of the IOPs may be possible,\textsuperscript{94} not just the depth-integrated IOPs that are typically found with inversion algorithms.

19.2.5 Nutrient and chlorophyll samples

Nutrient and chlorophyll data were collected for the West Florida Shelf in November 1998 from the ECOHAB Process Cruise and the MOTE Marine Laboratory Cruise. Whole water samples were filtered onto GF/F glass-fibre filter pads and stored on liquid nitrogen until extraction. The extraction of pigments was performed using a 98%:2% methanol: ammonium acetate solution. HPLC was performed on the extracts collected 16–19 November 1998 by MOTE Marine Laboratory. MOTE Marine Lab then subjected these samples to chemical taxonomy (Chemtax) evaluation (Wright et al., 1991) to calculate the contribution of a given algal class to the total chlorophyll \( a \) concentration. This programme uses a steepest descent algorithm to find the best fit of algal class based on an initial presumption of pigment ratios for the predetermined classes. The Chemtax algal classes were designated as one of the following algal classes: dinoflagellates, diatoms, cyanobacteria, chlorophytes, cryptophytes (commonly found in low-salinity waters) or \( K. \) \textit{brevis}.

This study focuses on Charlotte Harbor, Florida, so the data were limited to the lower Charlotte Harbor region with the northernmost latitude being 26.688N and the southernmost latitude being 26.333N (Figure 19.2). Data were also limited to the westernmost longitude of 82.463W. The eastern boundary of the simulation is the 10 m isobath. Samples collected shoreward of this boundary were considered equivalent to the near-shore boundary of the simulation. All zero values in the data were converted to \( 1 \times 10^{-3} \) to avoid complications of division by zero. Chlorophyll concentrations less than \( 1 \times 10^{-4} \mu g l^{-1} \) were deemed below the detectable limit of 1,000 cells \( l^{-1} \) and these values were essentially considered zero. Negative correlations were found between salinity and chlorophyll \( a \) concentrations as well as salinity and nutrient concentrations suggested riverine outflows as the source. Note, all the Chemtax data are used strictly for validation, not for initialization.

To compare field data collected on the WFS, which is a three-dimensional environment, to a two-dimensional model, the data first had to be corrected for the curvature and ellipsoid nature of the earth. A function written by Gillis and Montes (2001) of the Naval Research Laboratory was used to estimate distance between geographical coordinates. Each station’s distance from the 10 m isobath could then be calculated by triangulation from the northernmost and southernmost points of the 10 m isobath line segment. This method is an adequate approximation for our needs since the relationship between bathymetry and distance from shore is nearly linear over most of the EcoHAB:Florida domain.

There are two types of model/data comparisons that we would like to show. The first is the prediction of a tracer, i.e. total chlorophyll and the second is the phytoplankton ecological structure resulting from a given forcing condition. These comparisons may be difficult if the simulated physical forcing and boundary conditions are not perfectly matched to the actual field conditions (Bissett et al., 2005). In this study,

\textsuperscript{94} The retrieval of vertically-dependent IOPs from \( R_{rs} \) is the subject of current research by the authors of this chapter.
differences in simulated and actual biomass were at times large, mainly resulting from
temporal and spatial dislocations of water masses (Bissett et al., 2005). In order to
evaluate the ecological structure of the WFS and the simulation, biomass differences
in the Chemtax data were removed by dividing the total chlorophyll concentration
measured on the shelf by the simulated total chlorophyll concentration. This was then
multiplied by the simulated functional group’s chlorophyll \(a\) concentration and was de-
noted by ECOSIM’ (ES’). This new value was then compared with the Chemtax total
chlorophyll \(a\) concentrations of each algal class. Algal class comparisons of ECOSIM
and Chemtax were evaluated according to Table 19.1.

Figure 19.2
Location of stations where whole water samples were collected on filter
pads and subjected to Chemtax analysis to determine the contribution of
phytoplankton species to total chlorophyll \(a\) concentrations.
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19.2.6 Sensitivity of mortality closure

In this model, the loss of phytoplankton biomass is driven by both grazing and lytic losses (which include mass dependent phages and apoptosis) (Steele and Henderson, 1992). The sensitivity of this model is evaluated based on this closure term. The grazing stress is modelled by the following equation such that it is a function of a minimum mortality rate multiplied by the logarithm of the total biomass of a functional group divided by the refuge population (Bissett et al., 2005):

$$ g_i = \text{mortality}_i \times \log \left( \frac{\text{PC}_i}{\text{refuge}_i} \right) $$  \hspace{1cm} (19.2)

where the grazing stress on phytoplankton functional group $i$, is equal to the mortality parameter for functional group $i$ (d$^{-1}$) multiplied by the log of the particulate carbon concentration ($\text{PC}_i$; mol C or mol C l$^{-1}$) of phytoplankton functional group $i$ divided by the refuge population (mol C) of function group $i$. The refuge population is the concentration of carbon below which there is no grazing or lysis and is set to 0.02 mol C for all species (note, carbon is the base currency in the model, all other phytoplankton mass terms, such as PON or pigments, are functions of the light and nutrient history of the functional group at each time/space location in the model (Bissett, 1997; Bissett et al., 1999b, 2004; 2005). This function assumes that the magnitude of biomass concentration is the best indicator of loss stress. The responsiveness of the model to the closure term was investigated by halving and doubling the grazing stress on the various phytoplankton groups as described in Table 19.2.

Table 19.1  Comparison of chemtax and ecosim algal classes used for evaluation of the model

<table>
<thead>
<tr>
<th>Chemtax algal class</th>
<th>ECOSIM algal class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dinoflagellates</td>
<td>Non-toxic dinoflagellates</td>
</tr>
<tr>
<td>Diatoms</td>
<td>Large + small diatoms</td>
</tr>
<tr>
<td>Cyanobacteria</td>
<td>Synechococcus</td>
</tr>
<tr>
<td>Chlorophytes</td>
<td>Prochlorococcus 1 + 2</td>
</tr>
<tr>
<td>K. brevis</td>
<td>K. brevis</td>
</tr>
<tr>
<td>Cryptophytes</td>
<td>n/a</td>
</tr>
</tbody>
</table>

Table 19.2  The grazing stress ($g$, d$^{-1}$) on each phytoplankton functional group for various model runs

<table>
<thead>
<tr>
<th>Simulation description</th>
<th>Prochl</th>
<th>Syne</th>
<th>Large diatoms</th>
<th>Small diatoms</th>
<th>K. brevis</th>
<th>Non-toxic dinoflagellates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full grazing</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
</tr>
<tr>
<td>Half grazing</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>Double grazing</td>
<td>0.020</td>
<td>0.020</td>
<td>0.020</td>
<td>0.020</td>
<td>0.020</td>
<td>0.020</td>
</tr>
<tr>
<td>Mixed grazing</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
<td>0.005</td>
<td>0.020</td>
</tr>
</tbody>
</table>

Prochl: Prochlorococcus 1 + 2; Syne: Synechococcus
19.3 Results

A previous comparison between simulated and satellite-derived optical properties focused on the days where there were good quality SeaWiFS images for the West Florida Shelf. The simulated optical properties have previously been evaluated (Bissett et al., 2005) and the results presented here are used to evaluate the biomass distribution among phytoplankton species as well as the sensitivity of the model to physical forcing, boundary conditions and model closure. The days chosen for this evaluation are 8 June and 8 November. There were very few days during autumn 1998 that provided clear satellite imagery; however, the chosen days provided data of significant ecological and meteorological events that were evident in the both the satellite and available in situ data. 8 June occurred during a simulated and sampled increase in biomass resulting from a loop current intrusion, which originated in the Panhandle region (Walsh et al., 2003; Weisberg and He, 2003); and 8 November was just after a significant pulse of freshwater from the Peace and Caloosahatchee rivers following the landfall of Tropical Storm Mitch.

19.3.1 8 June (DOY 159)

As we are simulating multiple tracers (89) which correspond to nutrients, pigments, dissolved organic stocks and particulate organic stocks, many of the state variables may be directly compared with in situ data measured on the ECOHAB cruise. Differences in the nitrate concentration between simulated and sampled measurement collected on the WFS were greatest 40 km from the 10 m isobath at a depth of 25 m (Figure 19.3A). The underestimation of simulated nitrate concentration offshore at depth is not surprising given the fact that these samples were measured in a what appeared to be recorded upwelling/Loop Current Intrusion event and may also be due to inaccuracies in the physical circulation of the model as determined from the related manuscript. Probably correlated with this upwelling event was the underestimation of simulated total chlorophyll concentration at the same offshore station (Figure 19.3B).

Simulated silica was also underestimated near-shore at depth of 5 m and 10 m (Figure 19.4A). This may have been a result of pulse releases from terrestrial sources in April-May that were not simulated in this model (Figure 19.1). In one case, the simulation returned a value where the ECOHAB value was essentially zero. Inorganic phosphate concentrations were negligible offshore compared with near-shore concentrations (data not shown). Unfortunately, data revealing the phytoplankton composition on the WFS in June was not available for analysis. There was a large simulated intrusion event, which had similar nutrient and chlorophyll stocks (Figure 19.5A) as the measured event described in Figure 19.3. However, these stocks were located deeper and more offshore than the peaks in the measured data (50 m isobath). The simulated results suggest that the deep offshore waters were dominated by large and small diatoms, followed by Synechococcus and prochlorophytes (Figure 19.5A). In a recent publication, the modelled results of a nitrate rich intrusion of slope water on the WFS in June also produced a phytoplankton response, dominated by microflagellates.

Satellite-derived detritus and CDOM absorption (which in total is CDM), total chlorophyll and backscatter (Figures 19.6A, 19.6C, 19.6E respectively) on 8 June 1998 averaged over the entire domain (black line) and the Charlotte Harbor line (blue line) showed slightly elevated near-shore values with a declining gradient offshore. The slight elevation in near-shore values is indicative of a riverine source that was not simulated.
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Figure 19.3
Differences and percentage differences in A, nitrate concentrations; B, total chlorophyll concentrations by depth between simulated and sampled values at ECOHAB station 46, located approximately 40 km from the 10 m isobath, in June 1998, displaying an underestimation of nitrate offshore at depth. Negative differences represent an underestimation of chlorophyll a by the simulation.

Open circles, difference in ES and ECOHAB; filled circles, percentage difference.
Figure 19.4
A. Differences and percentage differences in silica concentrations by depth between simulated and sampled values at ECOHAB station 51, located approximately 6 km from the 10 m isobath in June 1998, displaying an underestimation of silica near-shore (note that in one instance, open square, EcoSim returned a value where the ECOHAB value was effectively zero).
B. Differences in silica concentrations by depth between simulated and sampled values at ECOHAB station 51 in November 1998, displaying an underestimation of silica near-shore.
Figure 19.5  
A, contour plots of the simulated total chlorophyll $a$ concentration attributed to each of the seven phytoplankton species and the sum of all the phytoplankton classes for DOY 159 – 8 June 1998.  
B, contour plots of the simulated total chlorophyll $a$ concentration attributed to each of the seven phytoplankton species and the sum of all the phytoplankton classes for DOY 312 – 8 November 1998.
Simulated and satellite-derived IOPs on the WFS.
A, total chlorophyll concentration (mg chl m\(^{-3}\)) on 8 June 1998, showing the average of the 30 lines transect, ±1 standard deviation of the mean of 30 lines, the mean of lines 22–30 (Charlotte Harbor), simulated absorption 5 m average for the full, half, double and mixed grazing stress runs.
B, total chlorophyll concentration (mg chl m\(^{-3}\)) on 8 November 1998 for the WFS.
C, detritus and CDOM absorption [\(a_{CDM} 412\) nm (m\(^{-1}\))] on 8 June 1998.
D, detritus and CDOM absorption [\(a_{CDM} 412\) nm (m\(^{-1}\))] on 8 November 1998.
E, backscatter (m\(^{-1}\)) on the WFS on 8 June 1998.
F, backscatter (m\(^{-1}\)) on the WFS on 8 November 1998.

(Bissett et al., 2005). Satellite estimated \(R_s\) on 8 June displayed an onshore to offshore gradient. Simulated \(R_{ss}\) (412 nm, 443 nm, 555 nm) also displayed an onshore to

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offshore trend (Figures 19.7A, 19.7C, 19.7E respectively). (The rise in the near-shore simulated values of $R_s$ compared with the offshore values is related to the impact of the simulated bottom reflectance in the shallow waters on the water-leaving radiance signal.) The relative success in simulating the satellite-estimated IOPs and AOPs during this time period results from the fact that the waters of the WFS at this time of the year approximate classical Case 1 waters, where the IOP and the AOP formulations of the simulation and satellite algorithm most closely match each other.

19.3.2 8 November (DOY 312)

After the passage of Hurricane Georges in late September of 1998, Tropical Storm Mitch (downgraded to a tropical storm from a hurricane just before moving onshore) made landfall on the west coast of Florida near Naples on 5 November 1998. The Page Field Airport in Fort Myers, Florida, reported 6.05 inches (15.4 cm) of rainfall on 5 November leading to large freshwater fluxes from the Peace and Caloosahatchee Rivers (Figure 19.1; W.P. Franklin Lock and Dam (S79)) over the course of several days. The ocean-colour impacts of these freshwater flows may be seen in the satellite derived chlorophyll, absorption and backscatter, which displayed a marked on-shore to off-shore gradient (Figures 19.6B, 19.6D, 19.6F respectively).

Simulated IOPs displayed a similar onshore to offshore gradient. Chlorophyll concentrations were elevated near-shore for the simulated model runs. The full grazing stress simulated chlorophyll concentration for the uppermost 5 m of the water column were within one standard deviation of the SeaWiFS mean across the shelf (Figure 19.6B). The half grazing stress run exceeded this threshold near-shore but was within it offshore; the double grazing stress was within this threshold at the near-shore boundary but fell slightly below it offshore.

Satellite-derived $a_{CDM}(412)$ was elevated near shore, and appeared to be the direct result of riverine CDM; the simulated results for the average of the top 5 m of the water column also displayed this trend. The satellite-derived absorption was elevated near-shore and declined offshore (Figure 19.6F). The simulated backscatter at 555 nm followed the same trend; however, the simulated values were slightly lower than the satellite estimates in all cases (although these simulated values are within one standard deviation of the mean). The overestimation of simulated backscatter might have resulted from the lack of sediment resuspension in the model, or perhaps surface boundary layer effects resulting from the high wind conditions surrounding the passage of the tropical storm.

SeaWiFS-derived $R_s(412)$ displayed a decrease from onshore to offshore with the greatest reflectance approximately 8 km from the 10 m isobath. Simulated $R_s(412)$ at the surface was lowest near-shore and increased offshore yet was below one standard deviation of the mean across the shelf (Figure 19.7B). Satellite estimated $R_s(443)$ was elevated near-shore with a maximum reflectance value approximately 8 km from the

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Simulated AOPs on the WFS. 

A, remote sensing reflectance ($R_{rs}$ 412 nm) on 8 June 1998 for the WFS showing the average of the 30 lines transect, ±1 standard deviation of the mean of 30 lines, the mean of lines 22–30 (Charlotte Harbor), simulated at the surface for the full, half, double and mixed grazing stress runs showing a fairly good match between estimated and simulated results.

B, $R_{rs}$ (412 nm) on 8 November 1998.

C, $R_{rs}$ (443 nm) on 8 June 1998.

D, $R_{rs}$ (443 nm) on 8 November 1998.

E, $R_{rs}$ (555 nm) on the WFS on 8 June 1998.

F, $R_{rs}$ (555 nm) on 8 November 1998.

10 m isobath (Figure 19.7D). Simulated surface values of $R_{rs}(443)$ were lowest near-shore and increased offshore yet were below one standard deviation of the mean across the shelf. Satellite derived $R_{rs}(555)$ values were elevated near-shore and declined offshore (Figure 19.7F). Simulated surface values of $R_{rs}(555)$ were underestimated near-shore where they were below one standard deviation of the mean; however, they were within
this range offshore. The trend in $R_n$ values of increasing towards shore for all wave-
lenghts, in spite of both the increase in satellite estimated and simulated $a_{CDM}$
resulting from terrestrial inputs of CDM, nutrients and particulate biomass, suggests
that backscatter at all wavelengths was underestimated. Higher scattering by either
sediments, or other surface induced effects, resulting from high winds would drive an
increase in water-leaving photon densities even as absorbing optical constituents are
increasing. As the satellite IOP and biomass algorithms used in this study are based
on relative water-leaving radiance, not absolute radiance, these differences are masked.
However, these examples demonstrate that ratio algorithms that produce absorption
estimates may work fine for some Case 2 coastal applications, but that scattering re-
trieval algorithms and the resultant $R_s$ calculation may be more difficult to develop
and validate without a better formulation for total scattering and backscattering.

Nutrient concentrations and filter pad samples for HPLC and Chemtax analysis
were collected on the WFS by the ECOHAB Process Cruise during its mid-Novem-
ber cruise and processed by Mote Marine Laboratory. For the near-surface stations in
the Charlotte Harbor region, observed differences between simulated and sampled total
chlorophyll were more dramatic near-shore (Figure 19.8). The simulated total chloro-
phyll concentrations were greater than the observed concentrations within 12 km of
the 10 m isobath for surface and near-surface stations. Biological factors, such as the

![Figure 19.8](image_url)

**Figure 19.8**
Difference and percentage difference between simulated total chlorophyll $a$ concentrations (μg l$^{-1}$) and Chemtax analysis of total chlorophyll $a$ concentrations attributed to phytoplankton classes for near-surface stations outside Charlotte Harbor in November 1998. Negative differences represent an underestimation of chlorophyll $a$ by the simulation.
concentration of chlorophyll per cell, which are a function of temperature, nutrients, and the light history of the phytoplankton population, may have played a role in the observed versus simulated chlorophyll differences. An additional role in the errors between the satellite observations may have occurred because of inaccuracies in the SeaWiFS OC4 algorithm in near-shore waters, which has difficulties with high turbidity and high dissolved organic matter. However, this overestimation of total chlorophyll compared with both in situ and satellite estimates may also be attributed to the physical simulation, because the first pulse event (DOY 267) was forced downward and offshore but then retreated back upwards and collided with the second pulse event on DOY 309 generating an additive effect (Bissett et al., 2005). The removal of the first pulse (data not shown) produced much better agreement with the observed satellite and in situ validation data.

While the exact cause of these errors in the near-shore region are unquantifiable given the nature of the physical solution, other satellite validation data (e.g. CDM) also suggest an over-estimation resulting from the accumulation of two pulse events at the same physical location.

ECOHAB data collected near Charlotte Harbor in mid-November revealed a salinity and chlorophyll fluorescence signature just outside the barrier islands, shoreward of the 10 m isobath (Figures 19.9A, 19.9B respectively). These signatures had characteristics of freshwater origin such as a diminished salinity and sigma-t (∼20–20.5 kg m⁻³, data not shown) compared with surrounding waters. Samples were processed by Chemtax analysis to determine the algal classes present on the WFS. Samples from this near-shore region (<12 km from the 10 m isobath) attributed between 15% and 33% of the total chlorophyll a concentration to chlorophytes and cryptophytes (Figure 19.10A). Samples from approximately 12 km offshore of the 10 m isobath attributed 11% of the total chlorophyll a concentration to chlorophytes and cryptophytes. This suggests that the bioavailability of nutrients and/or organic material from low-salinity waters (commonly where these species are found) was potentially delivered by the rivers out on to the WFS. Offshore, differences between simulated and sampled total chlorophyll a concentrations diminished.

Differences in simulated versus sampled silica concentration were also more pronounced near-shore. Simulated silica concentrations were greatly underestimated compared with sampled silica concentrations at a station 6 km from the 10 m isobath (Figure 19.4B). As near-shore silica concentrations are representative of terrestrial fluxes, it appears that we may have underestimated either the nutrient concentrations of those fluxes or the total fresh water discharge. The impact of a relative underestimation of silica inputs would result in a reduction in the growth rates and accumulation of large and small diatom functional groups. Inorganic phosphate was also underestimated near-shore but to a lesser extent. Simulated nitrate concentrations were very similar to those sampled across the shelf (data not shown).

The photosynthetic pigments and carotenoids present in various combinations and concentrations in marine phytoplankton were explored by HPLC and Chemtax analysis in order to determine the abundance of the algal classes listed in Table 19.1 on the WFS in November. Diatoms dominated the near-shore environment with ~50% of total chlorophyll attributed to this phytoplankton species 2 km from the 10 m isobath (Figure 19.10A). ECOHAB recorded silica concentrations between 4 km and 6 km from the 10 m isobath of approximately 4–5 μg Si l⁻¹ probably corresponding to the high concentrations of diatoms in the near-shore environment. K. brevis was a prevalent phytoplankton species in the near-shore community constituting 31% of the total chlorophyll concentration at the 10 m isobath. The next most dominant algal class was made up of
Figure 19.10
A. Percentage of total chlorophyll \( \alpha \) concentration (\( \mu \text{g} \text{l}^{-1} \)) attributed to each phytoplankton class present in near-surface samples outside Charlotte Harbor as a function of distance from model shoreward boundary.

B. Percentage of total chlorophyll \( \alpha \) concentration attributed to each phytoplankton class present in near-surface samples outside Charlotte Harbor as a function of salinity.
chlorophytes and cryptophytes constituted 33% of the total chlorophyll concentration 3 km from the 10 m isobath. Further offshore, diatoms were the most prevalent species making up 56% of the total chlorophyll concentration 12 km from the 10 m isobath.

Simulated full grazing stress results displayed a near-shore phytoplankton population dominated by prochlorophytes, *Synechococcus* and non-toxic dinoflagellates, while 12 km from the 10 m isobath, non-toxic dinoflagellates were the dominant phytoplankton species (Figure 19.11A). Simulated offshore results at depth suggested the presence of a diatom bloom with elevated concentrations of prochlorophytes (Figure 19.5B). The mixed grazing stress results show a transfer of biomass between the non-toxic dinoflagellates and the *K. brevis* populations (Figure 19.11B). This is to be expected because the numerical descriptions between the non-toxic dinoflagellates and *K. brevis* are more similar than between the dinoflagellate species and other phytoplankton populations.

Alterations of the relative grazing rates between dinoflagellate function groups (Table 19.2) results in a transfer within a niche space between non-toxic and toxic dinoflagellates. The WFS autumn 1998 observations of Walsh et al. (2003) demonstrated a near-shore bloom of *K. brevis* in the presence of CDOM as well as a deep offshore bloom of diatoms, similar to the results shown here. If differential grazing within a dinoflagellate favourable niche is an important ecological interaction, then the results presented here suggest good agreement with the occurrence of HABs on the WFS in November 1998.

Interestingly, when the same Chemtax data set was evaluated by salinity instead of by distance from the 10 m isobath, different results are evident. Chemtax analysis revealed diatoms to be the dominant fraction of phytoplankton present on the WFS at the lower and higher salinity levels with up to 43% of total chlorophyll concentration at 32 PSU and 42% at 35 PSU (Figure 19.10B). *K. brevis* was the dominant species at 33 PSU with 38% of total chlorophyll concentration attributed to this species and cyanobacteria dominated at a salinity of 34 PSU with 34% of total chlorophyll concentration (μg l⁻¹).

After the removal of chlorophyll biomass differences, it is clear that the simulation greatly overestimated the concentration of total chlorophyll *a* attributed to dinoflagellates across the shelf (Figure 19.12A). The three instances of over-estimation shown in Figure 19.12A resulted from Chemtax estimates for dinoflagellates that were below detectable limits and were effectively considered zero. The simulation returned values for these locations and the difference between these values approach infinity and are denoted on the graph. The same comparisons were made for the amount of total chlorophyll *a* attributed to *K. brevis* (Figure 19.12B). The simulation generally underestimated the concentration of total chlorophyll assigned to by *K. brevis*. The exceptions were in the near-shore environment where the Chemtax results were below detectable limits and the simulation returned values. In one instance, the simulated *K. brevis* concentration was overestimated 12 km from the 10 m isobath. This probably resulted from the simulated biomass being pushed farther offshore after the second pulse whereas, the actual recorded *K. brevis* bloom hugged the coastline.

After the removal of biomass differences, the concentration of total chlorophyll *a* attributed to diatoms were generally underestimated by the simulation in the near-shore environment (Figure 19.13A). Differences between ECOSIM large and small diatoms and Chemtax diatoms were greater in the near-shore environment and diminished offshore. The concentration of total chlorophyll *a* ascribed to *Prochlorococcus*, after the removal of biomass differences, was generally overestimated by the simulation (Figure 19.13B). Differences between ECOSIM *Prochlorococcus* 1+2 and Chemtax chlorophytes were greater in the near-shore environment with diminishing differences offshore. The same scenario was evident for the concentration of total chlorophyll *a* concentration at-
Figure 19.11
A, percentage of full grazing stress simulated total chlorophyll $a$ concentration ($\mu$g l$^{-1}$) attributed to each phytoplankton class in near-surface samples outside Charlotte Harbor.
B, percentage of mixed grazing stress simulated total chlorophyll $a$ concentration attributed to each phytoplankton class in near-surface samples outside Charlotte Harbor. Standard error of mean (±1) is denoted by error bars.
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Figure 19.12
A, removal of biomass differences between simulated and sampled dinoflagellates in near-shore waters.

B, removal of biomass differences between simulated and sampled *K. brevis* in near-shore waters. Grey circles indicate that simulation returned a value where the Chemtax value was effectively zero.
Figure 19.13
A, removal of biomass differences between simulated and sampled diatoms in the near-shore environment.
B, removal of biomass differences between simulated prochlorophytes and sampled chlorophytes in the near-shore environment.
C, removal of biomass differences between simulated *Synechococcus* and sampled cyanobacteria in the near-shore environment.
tributed to *Synechococcus* (Figure 19.13C). Comparisons between ECOSIM *Synechococcus* and Chemtax cyanobacteria were greater at the near-shore boundary; however, seaward of 2 km from the 10 m isobath differences between simulated and sampled values were minimal. The simulated overestimation of dinoflagellates, *Prochlorococcus* and *Synechococcus* were mirrored by a relative underestimation of diatoms and *K. brevis*. Such a result may have been driven by an overestimation of the relative growth rates (caused by inaccurate estimations of nutrient or light uptake and assimilation) or an underestimation of the relative loss rates between the diatom and dinoflagellate species. It may have also been a function of the lower simulated concentrations of silica. As noted above, there was a significant underestimation of silica in the near-shore environment. This would have led to a smaller simulated growth rate, as well as biomass accumulation, by the diatom functional groups.

**19.3.3 Closure sensitivity**

The closure term of grazing stress was altered to demonstrate that minor adjustments in this one term could produce varying results in terms of the simulated phytoplankton composition (Figure 19.11B) and optical properties on the WFS (Table 19.3). As expected, increasing the grazing stress caused a decrease in the chlorophyll concentration across the shelf and vise versa for decreasing the grazing stress whereas the mixed grazing stress run displayed minimal differences compared with the full grazing stress run. Major differences were observed, as expected, in phytoplankton biomass with the varying grazing stresses on both 8 June and 8 November.

Observed differences in optical properties and phytoplankton biomass were greater in November compared with June for the various grazing stress runs. The differences in chlorophyll concentration between the full and half grazing stress runs were attributed to the increase in biomass of non-toxic dinoflagellates and diatoms displayed in the half grazing stress run (Figure 19.14). The mixed grazing stress run produced minimal differences compared with the full grazing stress runs for both chlorophyll concentration and backscatter, since the *K. brevis* functional group represented a small fraction of the total simulated biomass.

### Table 19.3 Percentage difference between IOPs and $R_s$ for the half, double and mixed grazing stress runs compared with the full grazing stress run

<table>
<thead>
<tr>
<th></th>
<th>Half vs full grazing stress</th>
<th>Double vs full grazing stress</th>
<th>Mixed vs full grazing stress</th>
<th>Half vs full grazing stress</th>
<th>Double vs full grazing stress</th>
<th>Mixed vs full grazing stress</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>8 June</td>
<td>8 June</td>
<td>8 June</td>
<td>8 Nov</td>
<td>8 Nov</td>
<td>8 Nov</td>
</tr>
<tr>
<td>$a_{COH}(412)$</td>
<td>-11</td>
<td>9.2</td>
<td>-1.7</td>
<td>-13</td>
<td>11</td>
<td>-3.3</td>
</tr>
<tr>
<td>Chlorophyll</td>
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<td>-39</td>
<td>1.7</td>
<td>54</td>
<td>-43</td>
<td>3.3</td>
</tr>
<tr>
<td>$b_5(555)$</td>
<td>15</td>
<td>-14</td>
<td>0.46</td>
<td>17</td>
<td>-18</td>
<td>1.2</td>
</tr>
<tr>
<td>$R_s(412)$</td>
<td>-10</td>
<td>11</td>
<td>-0.44</td>
<td>-7.9</td>
<td>12</td>
<td>2.0</td>
</tr>
<tr>
<td>$R_s(443)$</td>
<td>-16</td>
<td>23</td>
<td>-1.1</td>
<td>-13</td>
<td>22</td>
<td>0.73</td>
</tr>
<tr>
<td>$R_s(555)$</td>
<td>-17</td>
<td>27</td>
<td>-1.4</td>
<td>-15</td>
<td>26</td>
<td>0.19</td>
</tr>
</tbody>
</table>
The most dramatic effect of altering the grazing stress was observed in the ‘mixed grazing stress’ which doubled the grazing stress on the non-toxic dinoflagellates while simultaneously halving the grazing stress on *K. brevis*. Comparisons of the full versus the mixed grazing stress cases revealed significant differences (*p* < 0.05, using paired Student t-tests) in the dinoflagellate population at 0 km, 3 km and 12 km from the 10 m isobath, the *Prochlorococcus* 1+2 population at 0 km and 12 km from the 10 m isobath, the *Synechococcus* population at 0 km and 12 km from the 10 m isobath, and the *K. brevis* population at 0 km, 3 km and 12 km from the 10 m isobath (Figures 19.11A, 19.11B). No significant differences were observed for the diatom population.

The most noticeable result was a decline in the dinoflagellate population from the full to the mixed grazing stress with a corresponding increase in the *K. brevis* population. This ‘mixed grazing stress’ was specifically developed to show the sensitivity of the grazing stress on the phytoplankton classes on the WFS. By slightly altering this single term, it was possible to generate a near-shore harmful algal bloom.

### 19.4 Discussion

Ocean optics and phytoplankton ecology are intrinsically coupled. An accurate understanding and prediction of one without the other is impossible. This volume of papers testifies to these linkages. However, typical HAB simulations often simplify these processes to avoid the complexities involved with generating a solution to both
the optical and ecological dynamics of the coastal zone. In this chapter, these results suggest that it is possible to simulate both optics and ecology in a manner that provides feedback between light and nutrient harvesting, phytoplankton competition and spectral photon densities. The explicit coupling of these fields of research in this numerical simulation suggests that the simplification of equation (1) may be unnecessary in HAB research.

As with the related paper by Bissett et al. (2005), a critical aim of this work was to avoid the reductionist viewpoint of modelling, which focuses on a minimal set of parameters and interaction equations to match a specific validation data set. While it may not appear evident to those unskilled in numerical modelling, a large number of state variables does not equate to a large number of free parameters. In this study, the parameters of time-dependent change for the mass constituents are fixed from laboratory or field measurements. The only 'free' parameter is the grazing and loss term. The EcoSim model is an evolving set of interaction equations whose parameters change when there is a change in the interaction equations. In the methodology used here, the parameters are not altered to match any particular data set. Instead, this modelling study concentrates on trying to build a framework that addresses both ocean colour and ecology across transition zones (ecotones) and will therefore be more applicable to both coastal and open ocean solutions. The goal was to develop an ecological framework that may be nested into larger physical models without constantly altering parameters for different geographical or ecological regimes.

As mentioned in the methods, the model results were in equilibrium with the physical solution, and the solution was generated for three simulated years prior to the analysis of the results. There were no numerical transients or ‘limit-cycle’ behaviours. Therefore, the ecological and optical results from this simulation are directly dependent on the physical circulation model. The WFS is a four-dimensional system \((x, y, z, t)\); He and Weisberg, 2002a, 2002b; Walsh et al., 2001, 2002), and its representation by a reduced-dimension circulation system \((x, z, t)\) introduces uncertainties in the comparisons of simulated data with \textit{in situ} data. A direct correlation study is thus difficult because the physics and boundary conditions drive the zero- and first-order solutions, where zero order is defined as the initial state and boundary conditions, and first order as the advective and diffusive fluxes. The ecological and optical solutions are second-order time-dependent problems that require accurate solutions to the zero- and first-order problems before exact comparisons of the ecological results may be made to geographically certain validation data. Significant errors in the physics and boundary conditions will cause errors that may not be the fault of the ecological coding. This is a statement of fact, not an assignment of blame, and is mentioned only to remind readers of the limits of the measurements of ‘success’ in any ecological modelling effort.

While not shown, the temporal evolutions of the results were very much as one would expect on the introduction of significant nutrients supplies at either the offshore or riverine boundary. We highlight two points in time (June and November), because (a) there are validation data not used in any formulation or assimilation of the model, and (b) these distinctly different time periods offer the ability to contrast different ecological conditions representative of this region, thereby demonstrating the model’s ability to cross ecological boundaries in time and space. While perfect comparisons between the simulated results and the field and satellite observations may not be possible, this modelling study helps us to focus on the ‘reasonableness’ of simulated biological, ecological and optical results. This focus allows us to reasonably comment on hypotheses of HAB formation on the WFS. One of the hypotheses offered, and
supported by this study, is that pre-existing small concentrations of *K. brevis* may interact with the terrestrial fluxes of nutrients to yield toxic concentrations of this HAB-forming species.

The complexity of this model allows for a full description of the non-stoichiometric nutrient interaction equations. This description shows the impacts of silica limitation on the diatom population, with a commensurate increase in DON and dinoflagellate populations. These non-toxic dinoflagellate populations exceed their toxic counterparts, because of faster growth rates and better light harvesting ability. The accumulation of toxic species occurs here because of differential grazing. Thus, this study suggests that non-stoichiometry (non-Redfield) nutrient dynamics may yield conditions favourable to dinoflagellate populations and that reduced grazing pressure on the toxic dinoflagellates may help lead to their accumulation. This study also suggests that a more definitive answer would be derived from a coupling an ecological/optical simulation to a fully four-dimensional physical modelling system of the WFS.

Errors in simulated versus observed results may also be attributed to the fact that chlorophyll concentration per cell varies with temperature, nutrient, light and species and that chlorophyll estimates from SeaWiFS can vary by a factor of 2 or more. An additional source of errors could be due to the fact that the OC4 chlorophyll algorithm was used in this study where CDOM and resuspended sediment had major contributions to the near-shore IOPs. Band-ratio algorithms are extremely useful due to their simplistic formulas; however, they are not optimized to distinguish CDOM from chlorophyll. The use of this algorithm in high-CDOM coastal waters has been examined and research has found that its accuracy deteriorates for near-shore waters with high DOM concentrations (Liew et al., 2001). Near-shore Case 2 waters were also somewhat more difficult to simulate as opposed to Case 1 waters. Some of the differences in the surface chlorophyll and $a_{\text{DOM}}(412)$ were attributed to the inability to simulate an along-shore flow (Figures 19.6B, 19.6D, 19.8); and some of the others attributed to the scattering of particles, or other high wind-driven effects, that were not included in the simulation (Figure 19.6E). However, one should not lose sight of the fact that we are discussing small relative errors between the ocean-colour estimates and the simulated values. This should be viewed as an achievement, and suggest that new standards for accuracy may evolve when IOPs are considered as part of the validation data suite.

This study also coupled radiative transfer equations (EcoLight) to link simulated IOPs directly to remote sensing reflectance, thereby providing a direct comparison of a reflectance result to a satellite reflectance measurement. This avoids the intermittent step required to validate against a satellite chlorophyll algorithm, which has its own inherent problems and errors. The fact that the results are on the same graph with scalar values on the $y$-axis should be cause for muted celebration, for this is validation at the physical level of photons and is within the standard deviation of the measurements. The fact that the backscatter and $R_s$ results are not as robust point to both the exclusion of an important optical constituents, e.g. resuspended sediments, and the fact that the very nature of Case 2 IOPs are still an area of very active research.

The taxa-specific results were not as strong, but they were encouraging. Clearly, the simulation under-estimated diatom concentrations and over-estimated non-toxic dinoflagellates. Part of the problem may have resulted from the inaccurate prescription of the shoreward boundary condition as the near-shore November silica con-
centrations were much lower than measured (Figure 19.4B). Another problem may have been taxa specific closure terms, and we could further explore the grazing parameter space to attempt to exactly match the relative contributions of the Chemtax estimates by further altering the loss terms. However, it is unclear that such tuning would render meaningful results, and it would be best to address the boundary conditions and physical model before attempting to tune the closure term to match the current data.

At first glance to the uninitiated, this might suggest that this model may be tunable to match specific results. However, this is not the message that is suggested here. The large number of state variables in this model provide for the closure of processes through multiple mass stocks that are directly measurable. For example, DOM and $a_{\text{CDM}}(412)$ are parameters that may be measured. Alteration of the grazing stress has direct impacts on these stocks and IOPs, thus the grazing stress and resulting processes are constraint by their inclusion in this model. Likewise, it was shown that the lack of silica flux results in a mismatch in total silica stocks, which limits the diatom growth rate and accumulation, which may be validated by Chemtax estimates as well as by nutrient measurements. In addition, a critical model validation is whether it performs well over different environmental forcing conditions. It may be possible to match simple validation data streams at limited locations in time and space; however, over broad time and space scales, simple PZN models tend to fail because the parameters used to match one data set will not yield robust answers in different environmental conditions. Thus, the example here of model simulations of the exact same parameter sets run over an entire year showing results under oligotrophic (8 June) and eutrophic conditions (8 November) gives confidence in the applicability of the results to understanding real ecological conditions and events.

The fact that the relative phytoplankton community structure and total stocks may be altered by model closure is (a) an exercise in the obvious, and (b) a demonstration that alterations in the loss terms resulting from upper trophic (and in the case of viruses, lower trophic) level dynamics are important and may be more difficult to simulate. However, this does not mean that predictive simulations of red tides are beyond our current means. In the case of the WFS, where it appears that *K. brevis* respond to total nutrient dynamics in a competitive regime of spectral light and multiple limiting nutrients, it may be possible to predict the probable conditions where *K. brevis* best occurs. This would provide the means to forecast probabilities, much like the weather forecast of rain chance percentages. As is evident here, such a probability forecast is critically dependent on the physical circulation model, as well as having accurate initial and boundary conditions for nutrients and organic stocks. The combination of new physical sensors, e.g. CODAR, in-water optical sensors and platforms, e.g. absorption and scattering sensors on gliders, and remote sensing tools and techniques, e.g. hyperspectral remote sensing, may provide the means to help initial and constrain the future nowcast/forecast HAB systems.

**19.5 Where do we go from here?**

In this study, an ecological model, which resolves the spectral harvesting of light by phytoplankton and the non-stoichiometric dynamics of nutrient cycling, is merged with the optical properties of the water column, such that the intersection between
biology and optical physics may be directly compared with satellite reflectance measurements. It is shown that within the constraints of the physical circulation and boundary conditions it appears that a reasonable representation of the K. brevis HAB on the WFS during autumn 1998 is produced, as well as the bulk chlorophyll, IOPs and AOPs. The successes can be listed as:

- Coupling of a fairly comprehensive phytoplankton ecological model to the prediction of inherent and apparent optical properties that provides feedbacks between light and nutrient assimilation and spectral photon densities.
- Validation of simulated bulk surface chlorophyll and IOPs with satellite-derived estimates with 1 standard deviation in Case 1 waters.
- Coupling of predicted inherent optical properties to a robust prediction of apparent optical properties to yield \( R_{sr} \) predictions that can be directly compared with satellite-measured photon densities, not just bulk properties that have errors associated with the satellite inversion error.
- The increased probability of K. brevis HAB formations on the WFS appears to be directly related to conditions that increase the total nutrient concentration on the shelf, i.e. a rising tide raises all boats, and differential grazing.

These successes are matched by some disappointments, which serve to point to areas of needed future research. Some of these are highlighted as:

- An accurate physical circulation model and boundary conditions is paramount to accurate simulation of phytoplankton, IOPs, AOPs and HAB formation.
- More research into Case 2 particle specific optical properties, including inorganic particles is needed in order to simulation IOP and AOP distributions in the near-shore environment.
- Numerical simulation of taxa specific phytoplankton dynamics may require additional research into the taxa specific loss processes (‘closure terms’), of the model.

In summary, optics and HABs should be studied and modelled as an integrated science, without resorting to simplifications that are unnecessary in light of this study. As mentioned at the start of this chapter, the complexity of the modelling approach chosen for a particular problem should be problem specific. In some cases, the use of optics as described here may not be as advantageous, e.g. Alexandrium in the Gulf of Maine, in the initialization and validation of numerical studies. In addition, there may be technical and financial constraints which limit the research to those numerical and modelling techniques that are more simply accomplished. However, the results here suggest that the study of ocean colour and HABs together (at least in this location) will provide greater insights into the biological and physical processes that yield these extreme events, as well as provide the data needed to initialize and validate future nowcast/forecast systems. These results suggest that optics may be explicitly linked to phytoplankton dynamics studies, and may actually hold the key to creating successful nowcast/forecast HAB systems.

References


Integration of ocean-colour remote sensing


Habwatch


Integration of ocean-colour remote sensing


AQ:
Due to repetition of subheading 19.2.2, subsequent subheading has been renumbered as 19.2.2 to 19.2.3 and so on. Please check for correctness.