CHAPTER 13

MODELING AND DATA ASSIMILATION

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1.0 Introduction

Coastal areas are by far the most complex and dynamic of all ocean regions. They are important zones for the accumulation and transformation of nutrients and sediments derived from terrestrial and atmospheric sources. These areas are also crucial fish nursery and foraging grounds and are home to the majority of ocean fish stocks that compose our fisheries Approximately 90% of the total marine fish catch is derived from continental shelf regions, an area comprising less than 8% of the total ocean area (). The proximity of the coastal ocean to terrestrial and fluvial influences complicates the underlying coastal ocean dynamics often associated with coastal regions, such as tides, coastal trapped waves, shoaling internal waves, upwelling, etc. Mankind has heavily influenced coastal regions by modifying freshwater influx patterns, altering nutrient and sediment fluxes from both fluvial and atmospheric sources, and overexploiting fisheries resources. One goal in understanding the dynamics of coastal regions is to use this knowledge to improve coastal management practices so as to reduce the impact of anthropogenic influences. However, gaining an understanding of the mechanisms important to answering a host of questions related to coastal ocean regions requires the coordinated use of a wide variety of data sets, of both satellite and *in situ* origin, and numerical models.

Remote sensing products are becoming increasingly available for coastal ocean applications (King et al., 2003). These products are typically derived from passive reflectance measurements (e.g. sea surface temperature from the Advanced Very High Resolution Radiometer, AVHRR; phytoplankton chlorophyll and primary production from the Sea-viewing Wide Field-of-view Sensor, SeaWiFS; and, Moderate Resolution Imaging Spectroradiometer, MODIS) or active microwave radar reflectance measurements (e.g. QuickSCAT for ocean surface wind velocities, and TOPEX and Jason-1 for ocean surface altimetric measurements). The capabilities and resolution of each of these satellite sensor/data products varies between coastal and open ocean regions. For passive remotely sensed data, the higher resolution Local Area Coverage (LAC) data are available for coastal regions, while open ocean region studies have access primarily to coarser resolution Global Area Coverage (GAC) data. While passive reflectance data sets from coastal regions are more resolved, Case-II waters associated with coastal zones makes deriving products, like surface chlorophyll, more difficult and prone to increased uncertainties due to higher concentrations of coastal-derived, optically-active scalars such as Colored Dissolved Organic Material (CDOM) and suspended sediments (Carder et al., 1999). Radar scatterometer (wind velocity) and altimeter (sea level topography) data sets involve separate issues related to data quality within coastal areas. Radar scatterometer estimates of wind, while well resolved in open ocean regions, are unable to resolve the small-scale wind field structures located near the coast, where wind measurements are required by circulation models to resolve processes such as coastal upwelling. Sea level topographic measurements are even more problematic because of the low spatial and temporal resolution of the data coupled with the noise issues due to tidal signals in coastal regions.

Because of the short time and space scales and complex dynamics associated with coastal environments, gaining further understanding of these regions remains difficult. As a result, methods are now being developed to merge satellite observations with models in an effort to understand and eventually predict the observed variability in these regions. However, many of the available coastal ocean satellite data sets have yet to be used in support of coastal modeling efforts (Table 1). The steps required to develop this capability are complex. The matching of observations to model variables, discerning between observational and modeling errors, properly constraining the model solutions with realistic forcing and boundary conditions and a host of other issues remain unresolved.

Table 1. List of presently available satellite-derived coastal ocean variables.

Measurement	Example Satellite Sensors	Used in Numerical Modeling	References on use of satellite data in modeling studies
Sea Surface Temperature (SST)	AVHRR, MODIS	Yes	Anderson et al., 2000; Fox et al., 2001; Di Lorenzo et al., 2004; Wilkin et al., 2004
chlorophyll *a*	SeaWiFS, MODIS	Yes	Prunet et al., 1996a,b; Semovski et al., 1995; Semovski and Wozniak, 1995; Di Lorenzo et al., 2004
Primary Productivity	SeaWiFS, MODIS	No	N/A
Chlorophyll Fluorescence	MODIS	No	N/A
Total Suspended Matter	MODIS	No	N/A
Organic Matter	MODIS	No	N/A
Coccolith Concentration	MODIS	No	N/A
Rainfall	TRMM	No	N/A
Photosynthetically	MODIS	Yes	Spitz et al., 2001

Available Radiation			
Suspended Solids	MODIS	No	N/A
Colored Dissolved Organic Matter (CDOM)	MODIS	Yes	Bissett et al., 1999a,b, Bissett et al., 2004
Wind Velocities	QuickSCAT	Yes	Fox et al., 2001
Sea Surface Topography	TOPEX, Jason	Yes	Fox et al., 2001; Di Lorenzo et al., 2004

The path towards making use of satellite observations for coastal ocean studies is marked with a host of model and algorithm applications, ranging from the radiative transfer models that are used to interpret the satellite observations to fully three dimensional (3D) coupled numerical circulation/bio-optical models. A wide array of numerical modeling activities presently makes use of satellite data to address specific coastal ocean-related questions. These models range in complexity from simple algorithms to complex systems of time and space dependent coupled partial differential equations.

Because coastal regions possess small space scale and short time varying processes and features, models play a crucial role in helping us understand the interplay between the various processes that contribute to the final observed dynamic fields. The scales of the processes that contribute to the evolution of the observed features are poorly resolved by *in situ* observations and in cloudy regions (such as coastal upwelling centers) even by satellite sensors. Numerical models are required to integrate the observations into a dynamic modeling framework in order to allow us to test hypotheses on coastal dynamics.

The status of modeling ocean processes has progressed rapidly in the last decade due to the increase in computer technologies; improved methods in computational fluid dynamics; improved knowledge in ocean circulation and biogeochemical dynamics; and, a large increase in the availability of remotely sensed data for model forcing and validation (Shchepetkin and McWilliams, 2003; Moore et al., 2004). Contemporary modeling efforts now use satellite data for a variety of purposes, ranging from model forcing fields to independent data sets for model validation (Robinson, 1996; Di Lorenzo et al., 2004; Wilkin et al., 2004). In coastal regions, where modeling efforts require high resolution data sets due to short time and space scales of coastal ocean processes, use of satellite data sets is crucial. In this chapter, the variety of ways that satellite observations are used to support modeling activities will be presented through an overview of present and anticipated future applications.

2.0 Diagnostic/Analytical Models

2.1 OVERVIEW OF DIAGNOSTIC MODEL DEVELOPMENT METHODOLOGIES

Satellite imagery has historically been used in coastal applications as a qualitative tool to characterize the spatial structure of coastal ocean features (Bernstein et al. 1977; Abbott and Chelton, 1991). Additional efforts to use these data focused on characterizing seasonal and interannual variability (Thomas and Strub 1989, 1990; Strub et al., 1990). By far, the dominant approach for using satellite and field data in a quantitative sense is to develop algorithms or models that make use of observed relationships (empirical algorithms) that require satellite or *in situ* data as input variables to estimate scalars or processes that cannot be measured from space. A crucial application of models using satellite observations involves using Radiative Transfer Models (Chapter 1) to estimate water-leaving radiance values near the ocean surface. These estimates are used—as shown below—to obtain estimates of optically active ocean scalars (chlorophyll *a*, colored dissolved organic material, etc.). There are a growing number of diagnostic models/algorithms presently available for use in the ocean remote sensing community (Table 2). Two applications of primary importance to coastal ocean ecosystem research are presented below.

Table 2. Diagnostic Models/Algorithms for Ocean Remote Sensing Applications on MODIS.

Estimated Scalar	Method	References
Chlorophyll *a* pigment	Empirical and Semi-Analytical Models	O'Reilly et al., 1998; 2000
Total Suspended Matter	Empirical Model	Gordon and Clark, 1980
Diffuse Attenuation Coefficient at 490nm	Empirical Model	Gordon and Clark, 1980
Chlorophyll Fluorescence	Analytical Model	Abbott et al., 1982; Abbott and Letelier, 1998
Colored Dissolved Organic Matter (CDOM)	Empirical, Semi-analytical Models	O'Reilly et al., 2000
Absorption Coefficients	Empirical, Semi-analytical Models	O'Reilly et al., 2000
Coccolith Concentration	Semi-analytical Model	Gordon et al., 1988
Primary Production	Empirical and Analytical Models	Iverson et al., 2000; Behrenfeld and Falkowski, 1997a; Howard and Yoder, 1997
Phycoerythrin	Semi-Analytical Model	Gordon et al., 1988

2.1.1 *Case 1: Ocean Chlorophyll a Estimates*

There are three distinct types of models to estimate ocean chlorophyll *a* using satellite reflectance data: empirical, semi-analytical and analytical. Of these, only the first two have been widely implemented. Empirical models use *in situ* observations of ocean chlorophyll *a* to develop a relationship between the apparent optical property (AOP) of spectral remote-sensing reflectance $R_{rs}(\lambda)$ or normalized water-leaving radiance $L_{wn}(\lambda)$ and chlorophyll *a* concentrations. A number of these models are presented and compared in O'Reilly (1998; 2000). For instance, the OC4 model (version 4),

$$\text{Chl } a = 10^{\left(a_0 + a_1 R + a_2 R^2 + a_3 R^3\right)} + a_4,$$

$$\text{where } R = \log\left(\max\left(\frac{R_{rs}(443)}{R_{rs}(555)};\frac{R_{rs}(490)}{R_{rs}(555)};\frac{R_{rs}(510)}{R_{rs}(555)}\right)\right), \text{ and} \qquad [13.1]$$

$$a_0 = 0.366; a_1 = -3.067; a_2 = 1.930; a_3 = 0.649; a_4 = -1.532$$

is a five parameter model that uses a 4th order polynomial to utilize the maximum band ratio, R, of three different waveband ratios of the spectral remote-sensing reflectance $R_{rs}(\lambda)$. The "maximum" function causes the model to switch to alternate band ratios when the other band ratios become lower. This band-ratio switching is how many of the CZCS pigment algorithms operate (O'Reilly et al., 2000). The majority of empirical models fit radiance band ratios (converted to either logarithmic or natural log scales) to *in situ* chlorophyll *a* data using a variety of functions such as power, hyperbolic, and cubic polynomials. These color ratio algorithms work best in Case I waters and do poorly in coastal Case II waters, where the increased number of optically-active constituents add to the complexity of the ocean color problem.

Semi-analytical models, the second model type, use relationships that relate Inherent Optical Properties (IOPs), typically backscattering $b_b(\lambda)$ and absorption $a(\lambda)$ coefficients, to $R_{rs}(\lambda)$ (Garver and Seigel, 1997; Carder et al., 1999) or $L_{wn}(\lambda)$. Semi-analytical models can be implemented as either forward or inverse applications. Forward model applications use observations of IOPs, either measured directly or estimated from relationships of IOPs and in-water distributions of optically-active compounds, such as chlorophyll *a* or CDOM, to calculate $L_{wn}(\lambda)$ or $R_{rs}(\lambda)$. Inverse model applications use observations of $L_{wn}(\lambda)$ or $R_{rs}(\lambda)$ to calculate chlorophyll *a* or CDOM concentrations (Hoge et al., 1999, 2001; Garver and Siegel, 1997; Siegel et al., 2003).

The majority of ocean color models have been developed for application to Case I waters, with few exceptions (Doerffer and Fischer, 1994; Carder et al., 1999). A more detailed presentation of the issues involved in applying these models to Case II waters found in coastal regions is presented in Chapter 6.

Several new computational techniques are now being used to refine and further develop the techniques for using satellite observations to estimate chlorophyll *a*. Chapter 9 of this book presents an overview of the various computational methods now under employ or development. The historical methodologies used to develop ocean color models are based upon either empirical formulations or subjectively defined relationships, such as waveband ratios. Artificial neural network techniques are now being used to retrieve chlorophyll *a* from $R_{rs}(\lambda)$ (Gross et al., 2000; Zhang et al., 2003) and to support the merger of ocean color data from multiple satellite missions (Kwiatkowska and Fargion, 2003). Only a few applications (Tanaka et al., 2000) have applied this technique to Case II waters. A recent global application of the semianalytical inverse ocean color model of Garver and Siegel (1997) uses a data assimilation technique called "simulated annealing" to optimize the IOP model parameters (Maritorena et al., 2002). The multiple satellite merger effort being supported by the National Aeronautic and Space Administration's (NASA) Sensor Intercomparison and Merger for Biological and Interdisciplinary Studies (SIMBIOS) project is using spectral data assimilation and simulated annealing techniques to develop a merged satellite data product. The utility of this new application is that it not only provides estimates but also provided the related uncertainties for a number of ocean color products.

2.1.2 *Case 2: Satellite-Based Models for Phytoplankton Primary Production*

Similar to models used to estimate chlorophyll *a* from spectral remote-sensing reflectance, $R_{rs}(\lambda)$, primary production models also fall into three distinct categories, empirical, semi-analytical and analytical. Empirical models that use chlorophyll *a* estimates to predict primary production were developed prior to the capability to measure chlorophyll *a* using satellites. Balch et al. (1989a) presents a history of the development of these initial model efforts (Table 3) that began with Ryther and Yentch (1957), and Balch and Byrne (1994) define the various problems encountered in estimating primary production from space.

Table 3. Models for phytoplankton primary production estimates.

Reference	Type[1]	Product	Required Data Input
Ryther and Yentch, 1957	E	photosynthetic rate at light saturation	chlorophyll *a*
Talling, 1957a, b	E	depth-integrated primary production	irradiance, I_K
Lorenzen, 1970	E	depth-integrated primary production	surface chlorophyll *a*
Smith and Baker, 1978	E	primary production	chlorophyll *a*
Smith et al., 1982	E	primary production	chlorophyll *a*
Brown et al., 1985	E	mean euphotic zone production	chlorophyll *a*
Eppley et al., 1985	E	depth-integrated primary production	chlorophyll *a*, temperature, day length
Platt (1986)	E	primary production	surface light intensity, chlorophyll *a*
Balch et al., 1989a	S-A	surface and depth-integrated primary production	pigments and temperature
Balch et al., 1989b	S-A	surface and depth-integrated primary production	pigments, temperature, and light
Behrenfeld and Falkowski, 1997a,b	S-A	depth-integrated primary production	temperature and chlorophyll

[1]**E**: Empirical; **S-A**: Semi-analytical; **A**: Analytical

Analytical models for calculating the depth-integrated, daily primary production, Π, [mg C m^{-2}] that resolve spectral, temporal and depth variability, termed WRMs for Wavelength Resolving Models (Falkowski et al., 1998), attempt to incorporate all of the physical, bio-optical and physiological processes that are involved in regulating net primary production. The explicit analytical model for

$$\Pi = \int_0^{z_{eu}} \int_{0hrs}^{24hrs} \int_{350nm}^{700nm} 12\,\Phi(\lambda,t,z)\; E_0(\lambda,t,z)\; a^*_{ph}(\lambda,t,z)\; d\lambda\; Chl(t,z)\; dt\; dz - \int_0^{z_{eu}} \int_{0hrs}^{24hrs} R(t,z)\; dt\; dz, \quad [13.2]$$

where $\Phi(\lambda,t,z)$ is the quantum yield for photosynthesis for available radiance [mol C (mol quanta)$^{-1}$], $E_0(\lambda,t,z)$ is the available incident spectral solar radiance [mol quanta m^{-2} s^{-1} nm^{-1}], $a^*_{ph}(\lambda,t,z)$ is the chlorophyll-specific absorption [m^2 (mg chla)$^{-1}$], $Chl(t,z)$ is the *in situ* concentration of chlorophyll *a* [mg chla m^{-3}], and $R(t,z)$ is the loss term for respiration [mg C m^{-3} s^{-1}] due to losses of fixed carbon from photosynthetic respiratory processes and nighttime respiration. The factor of 12 is a simple conversion term [12 mg C (mol C)$^{-1}$].

These models are termed semi-empirical because, as with the ocean color models, they require empirical relationships to provide model closure, in this case relationships that link the variables $\Phi(\lambda,t,z)$ and $a^*_{ps}(\lambda,t,z)$ to environmental conditions, such as light or temperature, that can be estimated by satellite observations or simulated/predicted using advanced numerical models (Moisan, 1993; Bissett et al., 1999b). For instance, Moisan and Mitchell (1999) developed a modified version of the WRM, similar to that developed earlier by Kiefer and Mitchell (1983), such that the quantum yield for growth and the chlorophyll absorption relationships were quantified using temperature and light dependent empirical relationships. Using these relationships, it is possible to obtain estimates of daily primary production using satellite-based measurements of sea surface temperature, chlorophyll and photosynthetically available radiance (PAR).

By integrating the WRM equation over the visible spectrum of available radiance the equation is modified into a Wavelength-Integrated Model (WIM). The actual integration of equation 13.2 must be carried out using the integration by parts technique, creating a more complex model equation. In practice this is not done (Falkowski et al., 1998). Instead, a daily primary production models is developed that is devoid of wavelength-dependent terms such that

$$\Pi = \int_0^{z_{eu}} \int_{0hrs}^{24hrs} \left(\varphi(t,z)\, PAR(t,z)\, Chl(t,z) - R(t,z)\right) dt\, dz \quad , \qquad [13.3]$$

where $\varphi(t,z)$ is the chlorophyll *a* specific quantum yield of photosynthesis for absorbed PAR [mg C (mol quanta mg chla m^{-3})$^{-1}$] (similar to the product of $\Phi(\lambda,t,z)$ and $a^*_{ps}(\lambda,t,z)$) and $PAR(t,z)$ is the Photosynthetically Available Radiance [mol quanta m^{-2} s^{-1}].

Further reductions can be made to these primary production models by creating a Time-Integrated Model (TIM), such that

$$\Pi = \int_0^{z_{eu}} \left(P^b(z)\, \overline{PAR}(z)\, \overline{Chl}(z)\right) dz \,, \qquad [13.4]$$

where $P^b(z)$ is the daily-integrated chlorophyll-normalized photosynthetic rate at depth that incorporates the respiration and quantum yield terms [mg C (mol quanta mg chla m^{-3})$^{-1}$], $\overline{PAR}(z)$ and $\overline{Chl}(z)$ are the depth-varying, time-averaged photosynthetically available radiance and chlorophyll a, respectively. This model can be further simplified by integrating over the depth interval between the surface and the depth of the euphotic zone. The resulting Depth-Integrated Models (DIMs) become simplified to the level that the equations fall into the category of the numerous other empirical-based models from earlier efforts (See Table 3). A round-robin comparison of the ability of a number of primary production models based upon surface chlorophyll, temperature, and irradiance is presented by Campbell et al. (2002).

The majority of the ocean phytoplankton primary production models, if not all, are based upon tedious, primarily subjective, efforts to develop relationships that utilize satellite-derived observations of key environmental variables such as surface chlorophyll, temperature, and radiance. As with the development of ocean color algorithms, new applied math and computational techniques are becoming available that offer new avenues for creating more sophisticated—though likely more complex—phytoplankton primary production models. Some of these applications include neural networks, genetic algorithms, genetic programming, and fuzzy logic (See Chapter 9), and the host of available data assimilation techniques. With the establishment of high quality primary productivity data sets (Balch et al., 1992), development of more accurate and sophisticated productivity models are now under development.

3.0 Deterministic Models

Beyond the realm of diagnostic models or algorithms that are used with satellite data sets to estimate ocean variables such as chlorophyll *a* are the more sophisticated dynamic models that have been developed to characterize the time evolution of ocean variables. These models are comprised of systems of coupled ordinary or partial differential equations and are solved through the use of numerical integration techniques and high performance computers. Several reviews (Franks, 1995; Hofmann and Lascara, 1998) present overviews on the variety of interdisciplinary, coupled circulation/biological models that have been used for marine ecosystem research. These modeling efforts range from simple time-resolved (spatially-homogeneous) box models, to depth-resolved, one-dimensional (1D) models, to fully integrated coupled three-dimensional (3D) circulation/biogeochemical models.

A wealth of biogeochemical models have been developed for open ocean regions such as Ocean Weather Station Papa (Fasham, 1995; Antoine and Morel, 1995; McClain et al., 1996; Signorini et al., 2001), Burmuda-Atlantic Time-series Station (BATS) region (Fasham et al., 1990; Doney et al., 1996; Hurtt and Armstrong, 1996; Spitz et al., 1998; Hurtt and Armstrong, 1999; Bissett et al. 1999a,b; Spitz et al., 2001), Equatorial Pacific (Christian et al, 2002a,b), and the Northeast North Atlantic (Fasham et al., 1999). The majority of these efforts were in support of the recent scientific program called the Joint Global Ocean Flux Study (JGOFS) that focused on developing an understanding of the processes controlling carbon and nitrogen fluxes in the open ocean in order to close the carbon and nitrogen budgets in these regions.

3.1 BOX MODELS

Box models continue to play an important role in addressing specific coastal ocean science questions, especially those related to carbon and nutrient fluxes (Gordon et al., 1996), and they support the development of more complex (1D and 3D) models by providing a simple numerical environment to test new model formulations (Moisan et al., 2002). Also included in the box model category are the bulk mixed-layer models applications of Fasham et al. (1990) that have been successfully applied to several data assimilation studies in open ocean regions (Spitz et al., 1998, 2001). Box models have historically been used in coastal regions as tools to study ecosystem and trophic level interactions (Hofmann and Lascara, 1998, Olivieri and Chavez, 2000), biogeochemical cycling between deep and surface waters of the ocean (Broecker and Peng, 1982) and volume, salt and heat conservation in coastal embayments and larger inland seas (Pickard and Emery, 1990). The latter effort uses simple mass balance equations for salt and water to derive information on turnover time scales or residence times for coastal estuaries and bays. These residence time scales are an important parameter for estimating the fraction of carbon and nutrient fluxes from fluvial sources that reach the coastal ocean (Nixon et al., 1996). Because present coastal ocean models do not resolve these small estuaries and bays and forcing fields for coastal inputs of nutrients and carbon are limited to regions not affected by tidal influence, estimates of these turnover time scales are important for linking the fluvial nutrient and carbon fluxes to the coastal models at the appropriate level.

3.2 ONE-DIMENSIONAL (VERTICAL) BIOGEOCHEMICAL MODELS

The primary forcing conditions that control the time evolution of biogeochemical processes in many of the regions of the ocean occur through vertical processes such as advection and diffusion of nutrients, vertical attenuation of solar radiation and sinking of particles. While circulation and diffusion processes are three-dimensional in nature, it has been demonstrated (Gill and Niiler, 1973; Moisan and Niiler, 1998) that over large enough spatial scales, the seasonal variability of physical features such as temperature, salinity, nutrients, etc. is forced primarily through vertical processes. Many open ocean modeling efforts have made use of this quality to develop one-dimensional (1D), vertical models for studying open ocean biogeochemical processes (McGillicuddy et al., 1995; Doney et al., 1996; Bissett et al., 1999a,b). It is worthwhile to note here that the work of Bissett et al. (1999a,b) is the first to simulate both apparent and inherent optical properties.

While 1D models are ideally suited for open ocean applications, they have also been applied to several coastal regions to investigate processes such as dissolved organic cycling (Anderson and le B. Williams, 1998) and benthic denitrification and nitrogen cycling (Balzer et al., 1998) and plankton ecosystems for upwelling regions (Moloney, et al., 1991; Moisan and Hofmann, 1996). The application of 1D models to coastal biogeochemical studies (Moisan and Hofmann, 1996; Soetaert et al., 2001) requires additional physical constraints in order to resolve those processes, such as upwelling, that are not commonly encountered in open ocean applications, with the exception of open ocean upwelling areas such as the Equatorial Pacific (Friedrichs, 2001).

Vertical 1D biogeochemical models are composed of systems of coupled partial differential equations that govern the time and space distribution of the non-conservative scalars, such as nutrients, phytoplankton, detritus, dissolved organics, etc. The general form of this equation is written as:

$$\frac{\partial B}{\partial t} = \frac{\partial}{\partial z} K_z \frac{\partial B}{\partial z} - \frac{\partial (Bw)}{\partial z} - w_{\text{sink}} \frac{\partial B}{\partial z} - \tau_{\text{nudge}} (B - B_{\text{clim}}) + S_B , \qquad [13.5]$$

where B is a non-conservative quantity (one of the variables in the biogeochemical model), K_z is the depth-dependent, vertical eddy kinematic diffusivity, w is the depth-dependent vertical (upwelling/downwelling) velocity of the fluid, and w_{sink} is the vertical sinking rate of the biogeochemical components. An additional term τ_{nudge} is also used at times to specify the time scale over which the biogeochemical components are nudged back to the background climatologies of the individual model components, B_{clim}. The net local source and sink terms S_{B} can be prescribed to simulate processes such as di-nitrogen fixation, denitrification, or loss of material to higher trophic levels. One additional item to note is that the vertical advection term in coastal applications should be written in the flux divergence form so that the effects due to strong vertical divergence/convergence in the vertical velocity field ($\partial w / \partial z$) are appropriately accounted for and mass and volume are conserved.

Several applications of these 1D models focus on coastal ocean regions. For instance, Moisan and Hofmann (1996) use a food web model coupled to a multi-nutrient (nitrate, ammonia, silicate) biogeochemical model to compare the cycling of nitrogen in both an onshore and offshore region of the California Current System. Model results from 1D models are commonly used to assist in parameterization of 3D coastal models (Moisan et al., 1996; Vichi et al., 2003).

Efforts at modeling nitrogen budgets in the coastal regions are now coupling benthic biogeochemical models to pelagic biogeochemical models. An overview of the approaches used in pelagic and benthic biogeochemical model coupling is presented by Soetaert et al. (2000). Soetaert et al. (2001) developed a 1D model to study biogeochemical processes as part of the Ocean Margin Exchange in the Northern Gulf of Biscay (OMEX). In this study, the model resolves the vertical structure of both water column (NO_3, NH_4, O_2, Phytoplankton C and N, Detrital C, Detrital N, Zooplankton C, and Suspended matter) and sediment (NO_3, NH_4 and O_2) constituents. The addition of a vertically resolved sediment model, while providing important estimates on rate of nutrient regeneration and denitrification rates, has significant drawbacks due to the higher spatial resolution (mm vs m) required to resolve vertical sediment processes. For instance, in the Soetaert et al. (2001) modeling effort, the time step for the fully coupled sediment-pelagic model was 10 times slower than for the pelagic model alone. However, resolving these processes is especially critical in coastal modeling efforts because of the uncertainty in the total amount of denitrification that occurs in coastal regions. Inclusion of sediment processes gives models a capacity to predict the total source of inorganic nitrogen through sediment remineralization as well as to predict the amount of organic nitrogen lost through denitrification processes (Seitzinger and Giblin, 1996, Balzer et al., 1998).

Recently, Moisan et al. (2004) have used a fully coupled biogeochemical model with nitrogen, carbon and oxygen pathways (Figure 1) to study carbon and nutrient pathways in the California Current System as a tool to configure a fully 3D coupled circulation biogeochemical model (Stolzenbach et al., 2004). One of the important components of this effort was the development of a particle coagulation model. In addition, oxygen profile data were used to help parameterize the two competing processes of particle sinking and remineralization processes—a fast sinking, rapidly remineralizing material is similar to a slow sinking, slowly remineralizing material, in that both release nutrients back into the water column at a similar rate. As in the work of Oguz et al. (2000) and other studies, oxygen profiles play an important role in optimizing the values of the parameters that influence the vertical flux of carbon and nitrogen.

In the Moisan et al. (2004) model (Figure 2), the microbial loop dynamics from Spitz et al. (2001) with bacteria, dissolved organic carbon and dissolved organic nitrogen and an inorganic carbon cycling model with alkalinity and dissolved inorganic carbon (following Ocean Carbon-cycle Model Intercomparison Project [OCMIP] guidelines, Orr, 1999; Lewis and Wallace, 1998) were added to the pelagic model from Stolzenbach et al. (2004) which contained multiple nutrients (NH_4, NO_3), phytoplankton, a dynamic phytoplankton carbon to chlorophyll ratio (θ), zooplankton, small and large detrital nitrogen. In its present state, the model is able to fully resolve pelagic carbon and nitrogen processes, but a total of 15 model components are required. As more aspects of the coastal carbon are investigated the number of components is expected to grow significantly. For instance, these models continue to exclude phosphate cycle dynamics, yet the debate continues as to whether specific coastal regions are phosphate versus nitrate limited (Hecky and Kilman, 1984).

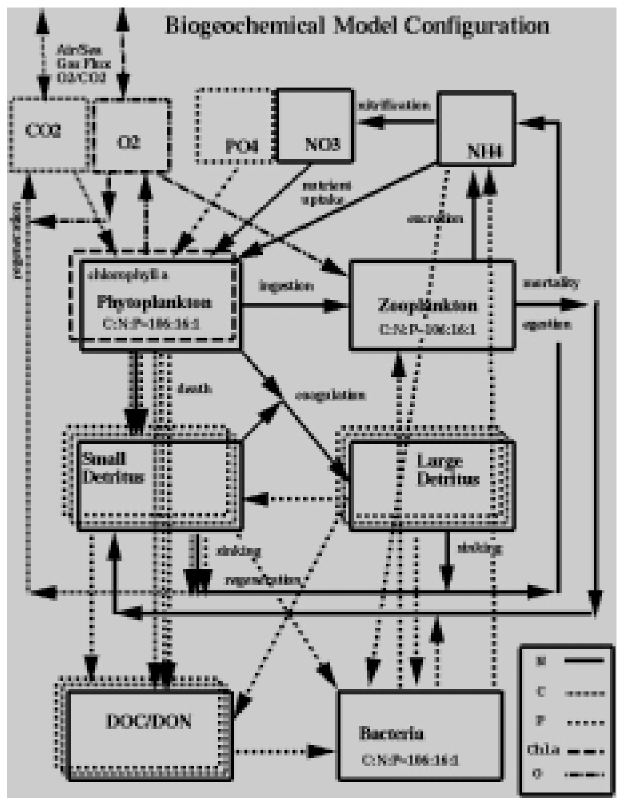

Figure 1. Present biogeochemical model configuration for U.S. West Coast Carbon Cycle modeling program. Not shown are the boxes for Oxygen, TIC, and Alkalinity. Carbon, Nitrogen, Phosphate, and Oxygen pathways are presently being resolved. All of the model pathways follow stoichiometric balances while maintaining variable C:N:P ratios for different model variables.

While it remains unlikely that 1D models will provide the ocean carbon cycling community with the final estimates that are required for closing the global carbon and nutrient budgets, 1D models will continue to play an important role in developing new model configurations and in parameterization of the more complex, 3D models.

3.3 THREE-DIMENSIONAL COUPLED CIRCULATION/BIOGEOCHEMICAL MODELS

Applications of three-dimensional (3D) ocean circulation models have typically been carried out under limited spatial domains, but the number of applications of the models has risen to encompass a significant fraction of the global continental margin domain (Figure 3). These 3D models are presently being configured to resolve circulation processes along many continental margin regions of the world ocean (Table 4). These coupled models generally employ circulation models that use the standard primitive equations to solve the time varying structure of the circulation fields (Haidvogel and Beckmann, 1999). The mode of integration primarily occurs using finite difference techniques, although other efforts have employed finite-element techniques (Lynch et al., 1996). In recent years, additional refinements to grid structures have incorporated grid nesting schemes that allow for enhanced resolution of the circulation processes in regions along the coast (Weingartner et al., 2002, Marchesiello et al., 2001 and 2002). Additionally, other coastal circulation models are using model outputs from basin or global scale model domains as input boundary conditions (Mantua et al., 2002).

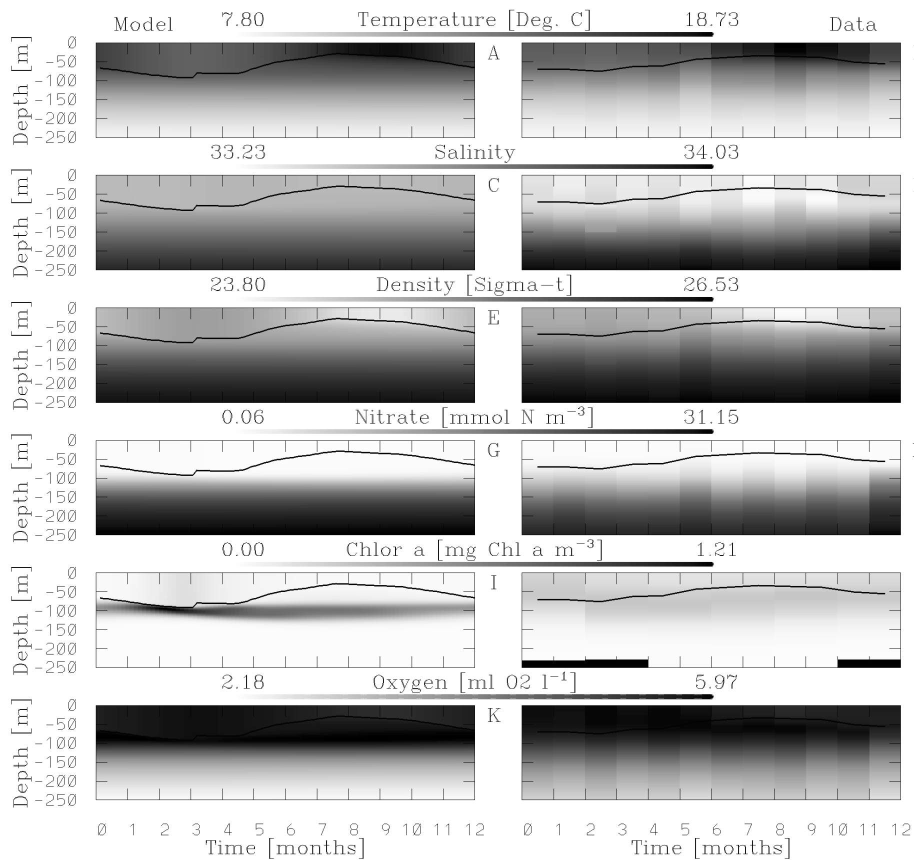

Figure 2. A comparison of the results (left panels) from a vertical (1D) coupled physical biogeochemical model to actual data (right panels) from an offshore region of the California Cooperative Fisheries Investigation (CalCOFI) domain (Moisan et al., 2004). For much of the world oceans, including coastal regions, the vertical structure of many of the biogeochemical features, such as nutriclines or chlorophyll maximums, are maintained by vertically dependent processes, such as light attenuation and vertical nutrient diffusion. The thick black line indicates the mixed layer depth.

The role of the physical circulation model in the coupled modeling system is to provide the biogeochemical model with information on the effects of vertical and horizontal advection and diffusion. In the 3D coupled models, the biogeochemical model is composed of a system of coupled partial differential equations that govern the time and space distribution of the non-conservative scalars, such as nutrients, phytoplankton, detritus, dissolved organics, etc. The general form of the equations is

$$\frac{\partial B}{\partial t} = \nabla \cdot K \nabla B - (\vec{v} + \vec{v}_{\mathrm{sink}}) \cdot \nabla B - \tau_{\mathrm{nudge}}(B - B_{\mathrm{clim}}) + S_B, \qquad [13.6]$$

where K is the eddy kinematic diffusivity, B is a non-conservative quantity (one of the seven variables in the biogeochemical model), $\vec{v}$ is the 3D velocity of the fluid, and $\vec{v}_{\mathrm{sink}}$ is the vertical sinking rate of the biogeochemical components. The velocity, $\vec{v}$, and kinematic diffusivity, K, fields are obtained from the 3D circulation model. The term τ_{nudge} is an optional nudging term that describes the rate that the biogeochemical components are nudged back to the background climatologies of the individual model components, B_{clim}, and S_{B} are the net local source and sink terms that describe the interlinking biogeochemical pathways between each of the model variables. The number of components used in the coupled 3D models has ranged from as low as 4 (Gregg and Walsch, 1992) to as high as 66 (Bissett et al., 2004).

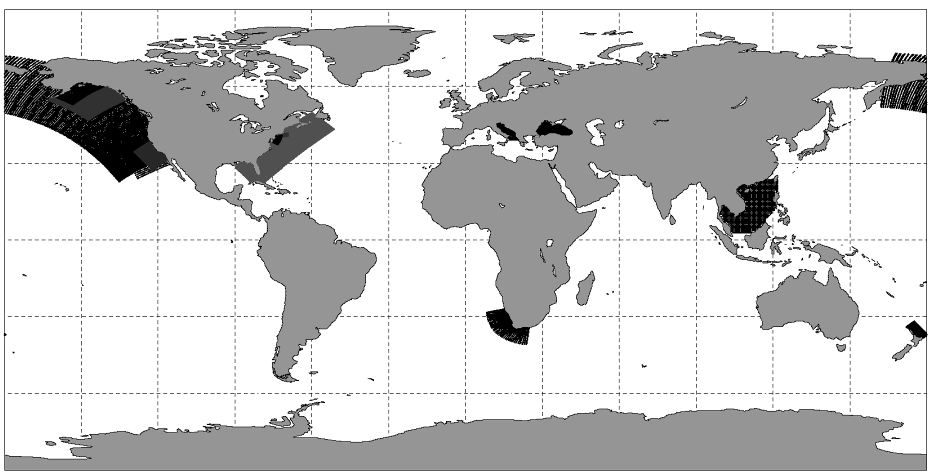

Figure 3. A global chart depicting a number of currently implemented coastal, coupled 3D circulation/biogeochemical models. See Table 4 for a complete listing of the modeling efforts represented within this figure.

Table 4. Coastal Three-Dimensional Coupled Circulation/Ecosystem Models.

Coastal Region	Physical Model	Ecosystem Model	Application	References
Alaska/U.S. West Coast	ROMS	NPZD	Fish Population Dynamics	Weingartner et al., 2002
Alaskan Gyre	ROMS	NPZD	Zooplankton Dynamics	Weingartner et al., 2002

U.S. West Coast	ROMS	Moisan et al., 2004	Biogeochemistry Carbon Cycle	Stolzenbach et al., 2004
U.S. East Coast	ROMS	Moisan et al., 2004	Biogeochemistry Carbon Cycle	Moisan et al., 2004
LEO-15 New Jersey	ROMS	ECOSIM	Bio-optics, Biogeochemistry	Bissett et al., 2004
California Bight	ROMS	Moisan et al., 2004	Ecosystem, Data Assimilation	Miller et al., 2000
South Africa	ROMS	Individual Based Model, NPZ	Small Pelagic Fish Recruitement	Mullon et al., 2002; Penven et al., 2001
South China Sea	Semtner	Fasham et al., 1990	Ecosystem, Nutrient Flux	Liu et al., 2002
Black Sea	POM	Complex, see: Oguz et al., 2002	Ecology, Biogeochemistry	Oguz et al., 1995 and 2002
Adriatic Sea	POM	Complex, see: Vichi et al., 2003	Nitrate Dynamics, Biogeochemistry	Vichi et al., 2002

3.3.1 *Biogeochemical Processes*

There are a host of processes that must be resolved in any 3D coupled model that is focused on simulating coastal ocean dynamics. At present, most of the coupled circulation biogeochemical applications address specific questions that relate only in part to the full coastal biogeochemical system. In order to correctly simulate the full biogeochemical system, even at a minimum or gross level of resolution, a number of critical biogeochemical model components must be included. The key components include: (a) pelagic ecosystem processes, (b) microbial loop processes, (c) multiple nutrients (NH_4, NO_3, SiO_4, PO_4, Fe), detrital (non-Redfield) dynamics, dissolved organic material (non-Redfield) dynamics, marsh and submerged aquatic vegetation (SAV) processes, benthic/sediment layer processes, and inorganic carbon dynamics that specifically follow Ocean Carbon-cycle Model Intercomparison Project (OCMIP, Orr, 1999; Lewis and Wallace, 1998) conventions/guidelines. With respect to coastal systems, it is important that the processes of nitrification and denitrification be specifically included. On the global scale, denitrification in coastal regions plays an important role in balancing the rate of ocean di-nitrogen fixation (Galloway et al., 1996). Also, processes in coastal regions play an important role in determining the amount of P that ultimately makes it way into the ocean interior. As mentioned in the 1D modeling section, the debate on the relative roles that P and N dynamics play in global ocean productivity on long time scales continues, and developing an appropriate coastal model to address this is crucial for correct carbon budget estimates on long as well as short time scales. One note of caution, creating models capable of simulating non-Redfield ratio dynamics—i.e. C:N:P ratios vary for DOM and POM depending of relative recycling/production rates—rapidly increases the level of complexity or number of model components with even a simple 8 component model (Figure 1). Care must be given to include only those processes that are crucial for accurate simulations in order to reduce the computational requirements and analysis complexity.

3.3.2 *Forcing and Boundary Conditions*

A wide range of forcing and boundary conditions are required to carry out reasonable and appropriate simulations of these 3D coupled models. The most difficult issue arising from trying to implement these models is open boundary conditions along the lateral open boundaries. Some recent efforts to develop improved open boundary conditions have been used by Marchesiello et al. (2001) in U.S. West Coast simulations. Other efforts have used larger basin scale circulation models to provide the necessary boundary conditions to force their coastal model using a 1-way nested configuration—information only passes from the large-scale model to the smaller scale coastal model.

Air-sea boundary conditions, besides requiring the general suite of heat and salt fluxes, also require estimates of airshed wet/dry deposition for specific model constituents such as NH_4 or POC/PON, and detailed parameterization for air-sea gas transfer. Because of the real lack of adequate data on all of the wet/dry deposition fluxes (Prospero et al., 1996), these have either been ignored or poorly estimated. Air-sea flux of gases is traditionally carried out using the “gradient method.” This method contains significant errors (factor of 2; Takahashi et al., 1997) due to wind speed parameterized estimates of the piston pumping velocity. In coastal regions, additional factors, such as increased surfactant levels, may contribute to the total error.

Forcing or boundary conditions at the coast should account for fluvial and consider groundwater (especially in karst plane regions) inflow into the continental shelf regions. Given that the populations of humans in the coastal regions continues to increase and land use practices continue to change and add stress to these regions, a number of factors should be considered when addressing this flux category. In a number of countries, freshwater flux recordings have been taken over the past tens of years and can be used to develop simple forcing conditions such as local climatologies. The situation changes when it comes to assessing the amount of fluvial Dissolved Organic Material (DOM), Particulate Organic Material (POM) or nutrient load that would ultimately reach the ocean margins. This issue is not a simple one to address and will require a significant level of effort to resolve. However, it is a crucial step in developing models that will be of practical use for land management issues.

4.0 Data Assimilation Efforts Using Deterministic Models

4.1 DATA ASSIMILATION FOR 1D BIOGEOCHEMICAL MODELS

The term “Data Assimilation” encompasses a wide range of applications. For instance, some aspects of data assimilation are simple data insertion or melding techniques where model solutions are nudged back into data compliance or blended with observations using techniques that guarantee dynamical consistency during periods when data are available (Robinson, 1996; Lozano et al., 1996; Robinson et al., 1996; Anderson et al., 2000; Anderson and Robinson, 2001). Other methods seek to minimize the errors between model solutions and observations (satellite or otherwise) by carrying out parameter or initial condition optimization. Efforts to use data assimilation to develop biogeochemical models have primarily focused on using data assimilation techniques for model parameter estimation (Table 5).

A large comparative data assimilation effort by Vallino (2000) tested the ability of various data assimilation methods to assimilate mesocosm experiment data into a marine ecosystem model. The results of this effort demonstrated a number of ongoing concerns facing implementation of data assimilation into ecosystem model development. Of the 12 data assimilation methods tested in this effort, no two solutions to the parameter set were similar. To date, there is no data assimilation method that has been accepted as being more appropriate than any other method. Indeed, no one method is available that can guarantee the parameter set solutions correspond to the parameter set that provides the global minimum error.

Table 5. Parameter optimization methods used in ecosystem models.

DA Method	References
Adjoint	Lawson et al. 1995, 1996; Matear and Holloway, 1995; Prunet et al., 1996a,b; Spitz et al., 1998, 2001; McGillicuddy et al., 1998
Markov chain Monte Carlo	Harmon and Challenor, 1997
Simulated Annealing	Matear, 1995, Hurtt and Armstrong, 1996, 1999; Vallino, 2000
Conjugate Direction/Gradient	Fasham and Evans, 1995; Vallino, 2000
Variational Assimilation	Prunet et al., 1996a,b
Simplex Algorithm	Vallino, 2000
Genetic Algorithm	Vallino, 2000

There are several important considerations that need to be addressed when assimilating data into models. A workshop to investigate the issues facing data assimilation of biological data in 3D coupled models identified a number of factors that must be dealt with for proper data assimilation applications (Robinson and Lermusiaux, 2000). With regard to the use of satellite data in data assimilation applications, there are three specific concerns that need to be addressed.

First, it is important to determine how the satellite estimated or *in situ* measured data equate to the model variables being simulated. This is especially true for ecosystem models where the definitions of model variables may be dramatically different from the working definition of the data being collected. For instance, models that attempt to simulate bacterial dynamics often represent bacteria in terms of the amount of nitrogen per unit volume [mmol N m^{-3}] whereas *in situ* data sets measure bacteria in terms of cell per unit volume (Spitz et al., 2001). Conversions between bacterial cell counts are not straightforward because at present there is no universally accepted value for converting bacterial cell counts into nitrogen or carbon biomass (Carlson et al., 1996). In addition, a number of studies have shown that up to 25% of the enumerated bacteria may in fact be prochlorophytes rather than the assumed heterotrophic bacteria (Sieracki et al., 1995; Carlson et al., 1996); and, it is now widely recognized that the metabolic state, dead vs. living vs. senescent (LeBaron et al., 2001), of individual bacteria cells varies widely with the majority of the cells being either senescent or dead.

With regard to the use of satellite data sets, the primary concern is in matching satellite estimates of chlorophyll *a* to estimates of phytoplankton nitrogen—the limiting nutrient and primary “currency” used within ocean biogeochemical models, e.g. Fasham et al., 1990. Early attempts of using nitrogen-based models to simulate *in situ* chlorophyll *a* simply assume constant C:Chl *a* [mmol C mg Chl a^{-1}] or N:Chl *a* [mmol

N mg Chl a^{-1}] ratios for carrying out the conversions to chlorophyll *a* concentrations (Hofmann and Ambler, 1988). In fact, the majority of ocean biogeochemical models in use today continue to use constant C:Chl *a* ratios (McClain et al., 1996; Signorini et al., 2001), though a number of modeling efforts have begun to include dynamic chlorophyll *a* pools (Doney et al., 1996; Spitz et al., 1998; Hurtt and Armstrong, 1999; Bissett et al., 1999a,b; Spitz et al., 2001). The wide variability of the phytoplankton chlorophyll *a* to carbon ratio (Geider, 1987) makes it an important parameter to resolve in order to carry out comparisons between model solutions and observational data sets. Only recently have modeling efforts included dynamic chlorophyll *a* to carbon ratios (Spitz et al., 1998,2001) for both ecosystem modeling and data assimilation application.

The second issue concerns the matching of model solutions to satellite observations. There are primarily two methods presently being used to achieve this. One method involves matching model-simulated variables, e.g. chlorophyll *a*, to satellite-derived values. Smith (1981) presents an integral approach to compare *in situ* profiles of chlorophyll *a*, $Chla(z)$ [mg Chl a m^{-3}], with satellite-derived estimates of ocean chlorophyll *a*, $Chla_{sat}$, such that

$$Chla_{sat} = \int_0^{Z_{90}} Chla(z) e^{-2\int_0^z K(z)dz} dz \Big/ \int_0^{Z_{90}} e^{-2\int_0^z K(z)dz} dz, \qquad [13.7]$$

where Z_{90} is the depth [m] above which 90% of the upwelling light field is generated, and $K(z)$ is the diffuse attenuation coefficients [m^{-1}]. An alternative, more sophisticated (but presently unimplemented) method is to directly simulate the IOPs, such as backscattering $b_b(\lambda)$ and absorption $a(\lambda)$ coefficients (e.g. Bissett et al., 2004), and use a forward optical model (e.g. Garver and Seigel, 1997; Carder et al., 1999) to predict the spectral remote-sensed normalized water-leaving radiance $L_{wn}(\lambda)$. The modeled quantities of $L_{wn}(\lambda)$ are then available for directly comparing against satellite remotely-sensed $L_{wn}(\lambda)$ values.

The third issue is related to differentiating between model and satellite errors. Both model solutions and satellite data have significant sources of error. Even direct comparison of model solutions and satellite data against *in situ* observations remains complex (Figure 4). This is because the errors associated with model solutions and satellite calibrations are highly variable in space and time. This is especially true for satellite data in coastal regions, where the presence of Chromophoric Dissolved Organic Matter (CDOM) and suspended sediments create Case II water conditions that ocean color models/algorithms perform poorly within, and where coastal ocean models are unable to resolve many of the smaller scale features and additional biogeochemical coastal processes. Any comparisons between model performance and satellite or *in situ* observations must be carried out using valid statistical techniques, and all comparisons should avoid the extreme temptation to subjectively note that the model solutions “look good” when compared to satellite or *in situ* observations.

4.2 ASSIMILATION OF SATELLITE DATA INTO COASTAL OCEAN MODELS

In principal, assimilating satellite data into coastal ocean models is no different than any other data type. Huge volumes of satellite data, however, normally require smoothing or sub-sampling to reduce the total number of observations for easier manipulation and for removing redundancies among closely spaced data when the model grid is coarser than the satellite data grid.

Additional considerations arise when carrying out spatial comparisons between data and model grids of multiple resolutions, as often occurs. A statistical approach is required to allow the model errors to be separated into locational versus quantity errors, the latter being more related to data assimilation cost function determination (Pontius, 2002).

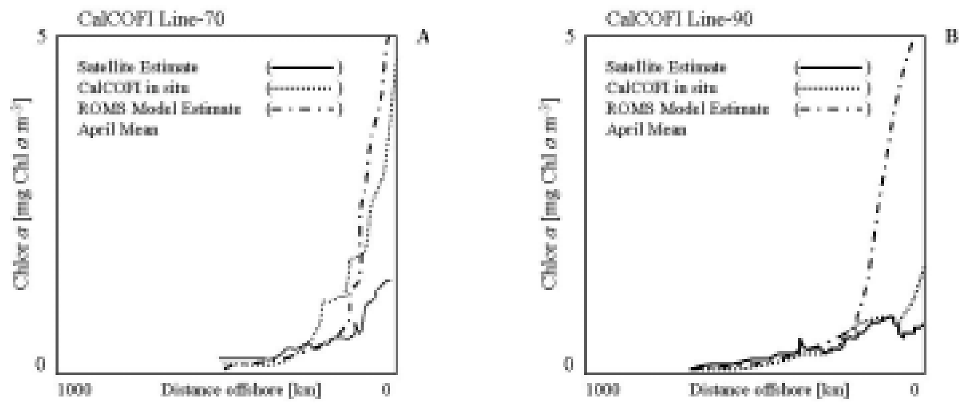

Figure 4. The April mean chlorophyll *a* estimates obtained from a coupled 3D circulation biogeochemical model is compared to SeaWiFS satellite estimates and *in situ* observations collected along two California Cooperative Fisheries Investigation (CalCOFI) lines. In the coastal regions, the 3D model estimates along the CalCOFI Line-70 (A) agree better with the *in situ* observations than do the SeaWiFS satellite estimates. The reverse is observed along the CalCOFI Line-90 (B).

Depending on the application of the assimilated solution, different techniques may be used to constrain the models (Bennett 1992; Wunsch 1996; Lermusiaux and Robinson 1999). These techniques are broadly grouped into “strong constraints” (where no artificial forcing terms are imposed on the dynamics) and “weak constraints” (where artificial forcing is allowed) formalisms. Strong constraints are more appealing when one wishes to diagnose the dynamics of an evolving flow according to the dynamics allowed by the model. They are also more useful when making forecasts, since the artificial forcing is not predictable. Weak constraints are more appealing when one wishes to make the most accurate maps of the fields. They are also useful in initializing forecasts.

Among the weak constraint techniques are ‘direct insertion’, where model values are simply changed to observed values at some time step, ‘nudging’, using a relaxation term to force the model over some time interval towards observed values, and ‘blending’, 'optimal interpolation' or 'Kalman filter', where model states and observed fields are melded together in suboptimal or optimal ways, sequentially at each timestep that has new data. One can also formulate the 'representer method' (Bennett, 2002) in a weak constraints formalism in which the artificial forcing field is determined for the entire state at each time step. More sophisticated techniques for predicting the error fields of the model, even non-linearly, have also been developed, such as the error-subspace estimation (ESSE) technique of Lermusiaux and Robinson (1999).

Among the strong constraints techniques are '4D variational assimilation' (4DVAR) in which a cost function (generalized data mismatch) is minimized based on assessing its curvature and directing the correction to the state vector downgradient until convergence is reached. This can be accomplished with the adjoint of the forward ocean model, which evaluates the gradient for the entire state vector, or with Green's functions, which evaluates the gradient for only a portion of the state vector variance, or with the Kalman smoother. The representer technique can also be formulated in a strong constraints framework.

4.2.1 *Case 1: CalCOFI and the Southern California Bight*

The Southern California Bight (SCB) encompasses part of the southern California Current System (CCS) and is an especially data-rich region because the California Cooperative Oceanic Fisheries Investigations (CalCOFI) Program has been collecting physical-biological data there for over 50 years (e.g. Chelton et al. 1982; Roemmich 1992; Hickey 1993; Roemmich and McGowan 1995; Hickey 1998; McGowan et al., 2003). The non-synoptic time and space resolution (roughly 1 month and 70 km, respectively, for a typical cruise track) of this *in situ* sampling, however, is inadequate to properly resolve the vigorous mesoscale circulation features in the region. And it is precisely these features that control the dominant biological and physical changes via localized upwelling cells, meandering fronts and filaments, and thermocline eddies (Strub and James, 2000; Swenson and Niiler, 1996).

Remotely sensed sea level height, SST, and ocean color provide a more detailed view of the region, but are limited in that they sample only surface features, have limited resolution, and do not extend right up to the coast. Combining the *in situ* and satellite data with data assimilation techniques in ocean models of this region is a perfect marriage of data and technique.

The CalCOFI field and satellite data has been used in strong constraints data assimilation strategies (a Green's function inverse method) to examine the short-term evolution of mesoscale features, e.g., within the time span of a single CalCOFI cruise (Miller et al., 2000; Di Lorenzo et al., 2004). With the advent of many new techniques for obtaining quasi-synoptic, high space and time resolution observations (e.g., CODAR estimates of surface currents, drifter platforms for salinity, atmospheric pressure and biological measurements, subsurface glider measurements of the upper ocean, etc.), it is of great importance now to develop procedures that can make use of this combined suite of observations to synthesize a complete picture of coupled physical-biological activity. An adjoint model 4DVAR approach with ROMS (Moore et al., 2004) is now being tested with CalCOFI and satellite data sets in the SCB. While adjoint data assimilation techniques have been widely used in 1D biogeochemical model applications, they have yet to be applied to 4D coupled models. This is primarily due to the large computational costs associated with carrying out numerous model runs.

Several practical issues of assimilating satellite data into the flow fields of the SCB were addressed in an identical twin experiment in which a model run was used to create synthetic data that are sampled and treated like observations (Figure 5c). The relative importance of using hydrographic data and TOPEX altimetry was assessed in these fits using a Green's function inverse method (Miller and Cornuelle, 1999). The ocean model was first run from an initial condition derived from an objective analysis of the synthetic hydrographic data. This forward run was then sampled at the data points to determine an initial model-data mismatch with the synthetic hydrographic data. The linear inverse method was then used to correct the initial conditions and the model was re-run from this new starting point (Figure 5a,b). Table 6 shows the linearly predicted error variance reduction and the actual variance reduction when running the fully non-linear model.

The correction using only hydrography as a constraint on the flow reduced the hydrographic error variance (model-data mismatch) by roughly 60%. The correction using both hydrography and TOPEX altimetry improved the mismatch with sea level only in the areas where no hydrographic data was available. It failed to improve the mismatch in the region with the synthetic hydrographic data, showing the importance of subsurface information on constraining the total flow field.

Smaller-scale structures that are not sampled by either sampling scheme could not be accounted for by the inverse solution. The inverse solution was only able to reconstruct the well-sampled larger-scale features of the eddy field, not the smaller scale eddies. These larger scale features were, however, dynamically important because they produced realistic large-scale flow fields which have predictive skill at leads of several months.

Table 6. Error variance reduction in identical twin data assimilation experiments

Expected reduction variance		**True non-linear variance reduction**	
CASE T, S (Fig 1a)			
Total	65%	Total	61%
Salinity	58%	Salinity	45%
Temperature	61%	Temperature	56%
CASE T, S, SSH (Fig 2a)			
Total	89%	Total	71%
Salinity	50%	Salinity	35%
Temperature	58%	Temperature	50%

4.2.2 *Case 2: New Jersey Long-term Ecosystem Observatory (LEO)*

Using circulation models to carry out ocean forecasts has been the goal of the U.S. Navy's Operational Forecast effort for some time. A recent review of the state of this effort is presented in a special issue of Oceanography magazine (Oceanography, Vol. 15(1), 2002). Research into developing methodologies for incorporation of real time data sets into these models is ongoing. As the Integrated Ocean Observing System (Ocean.US, 2002) continues to develop and *in situ* data sets become more readily available—especially in real-time, the need for and utility of coastal ocean forecasting capabilities will increase.

A coastal forecasting effort that uses satellite data and *in situ* coastal ocean observations from the Long-term Ecosystem Observatory (LEO) on the New Jersey coast has recently demonstrated the capability of a regional coastal ocean model to assimilate data and generate model forecasts in support of real-time adaptive sampling strategies (Wilkin et al., 2004). In this effort, the Regional Ocean Modeling System (ROMS) model, a 3D ocean circulation model, was used in conjunction with the U.S. Navy's Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS) to provide high resolution model solutions of the circulation field, and ocean temperature and salinity. The ocean circulation model region included the New York Bight and New Jersey shelf with an average horizontal grid resolution of 1 km and a higher resolved (300 m) grid region of 30 km by 30 km in the vicinity of the LEO observational area. Details on the configuration, forcing, and boundary conditions are presented by Wilkin et al. (2004).

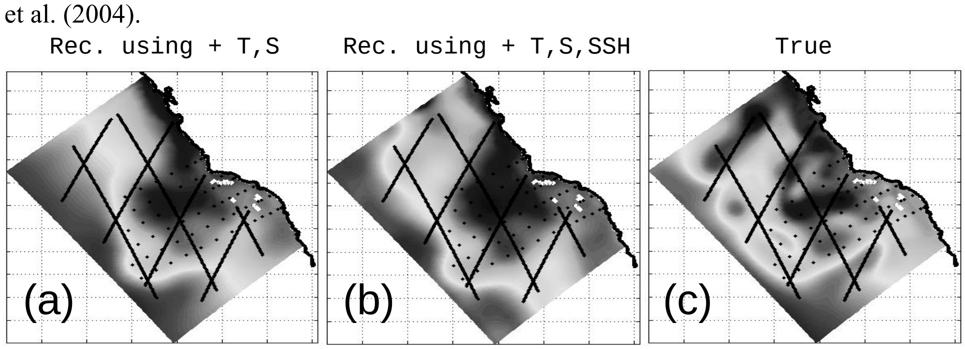

Figure 5. Sea level maps from an identical twin data assimilation experiment corresponding to a CalCOFI cruise. Three-week CalCOFI cruise sampling of hydrography is marked by dots. 10-day repeat cycle of TOPEX altimetry sampling is marked by solid lines. (a) Average sea level over the there week period for the model run from initial conditions corrected by the inverse technique assimilating only hydrography data. (b) As in (a) but but assimilating both hydrography and altimetric sea level. (c) The "true" sea level pattern from the base run. Note the small-scale structures in (c) that are unable to be measured by CalCOFI or TOPEX.

The model was used with real time data from the annual Coastal Predictive Skill Experiments that occurred between 1998 and 2001. The Coastal Predictive Skill Experiments were a series of modeling and field experiments that incorporated the model forecasts into the decision making processes for scheduling/developing the ship-based field survey for subsequent field campaigns. In addition to the shipboard data sets that provided temperature, salinity and density profiles from CTD deployments, high resolution and long-range radar (CODAR) systems provided surface current estimates, and satellites provided surface maps of temperature that were available for assimilation into the model. Additional observations of temperature from thermistors placed onto moorings, and horizontal current profiles from several bottom-mounted Acoustic Doppler Current Profilers (ADCPs) were used as independent observations to validate the model predictions.

Two data assimilation techniques, nudging and simple sub-optimal intermittent melding, were tested for generation of the 3-day forecasts that were made available to the oceanographic field survey team. Data nudging methods simply push the model solution towards the observations over some given time scale (e.g. equation 13.5). Data melding methods use weighted sums of the objectively mapped observations and forecasts to re-initialize the model at given periods in time. More recent data assimilation developments to ROMS now allow for use of adjoint and tangent linear data assimilation methods (Moore et al., 2004).

Because CODAR data sets only provide information on surface current, assimilation of these observations can introduce significant vertical shear into the horizontal velocity fields, and can severely hamper forecast skill. In order to reduce this impact, Wilkin et al. (2004) used a modified projection scheme based on the correlations between the CODAR surface data and the ADCP current profiles. This vertical extrapolation method provides a statistically based approach to extend the CODAR data sets throughout the water column and reduce the introduction of unwanted vertical sheer. While Wilkin et al. (2004) also assimilated satellite derived SST, the effect of assimilating surface scalar values such as SST may not be as critical as it is for assimilation of momentum data. In fact, SST observations have long been used in the modeling community for alternative air-sea boundary conditions when heat flux estimates are not available.

The use of real time observations to support ocean forecast efforts is a recent development for oceanographic research and field support applications. Of the two data assimilation methods tested by Wilkin et al. (2004) the assimilation by data melding provided model solutions with greater forecast skill. The introduction of increasingly sophisticated 3D data assimilation techniques (Moore et al., 2004), improved methods to adequately assimilate surface ocean observations, and increases in coastal ocean observations will support improvement of data assimilation applications in coastal regions, e.g. increased forecast skill and duration times.

5.0 Future Directions

As computational capabilities grow so too will the ability to carry out more effective modeling and data assimilation studies. However, a number of critical areas need to be further developed for coastal ocean modeling and data assimilation efforts to evolve to a level that can support operational and forecast applications.

Because of the complexity of coastal regions, modeling studies are crucial tools for the synthesis of available knowledge (read: data), for developing and testing new theories and challenging old paradigms, and for providing decision making tools to coastal managers. A coastal ocean observation program is currently being developed (Ocean.US, 2002) that call for the parallel development of coastal modeling efforts. The use of Observation System Simulation Experiments (OSSEs) needs to be encouraged for support of any observation development program effort. For instance, 3D coastal models have already been used to demonstrate the unlikelihood—due to prohibitively high costs—of using ocean moorings to estimate cross-shelf fluxes of carbon from coastal regions (Figure 6).

There is no doubt that for biogeochemical modeling and data assimilation efforts, data limitation will remain a reality. Even with successful implementation of an ocean observing system, the ocean will remain under-sampled. Because of this, care must be taken in development of any observational system so that it is used to provide the most benefit within the limited available funds. Modeling studies can provide insight in how such an observation system might be developed. There has been some discussion about the use of Observational Systems Simulation Experiments (OSSEs) and their role in validating data assimilation techniques under specific present or proposed observing systems. An additional role of these OSSEs should be to link them with data assimilation “twin experiments” to design an optimal observation system that uses a cost-function based upon both the error estimates and the actual costs (in dollars) for the specific observing system. The goal with such an exercise would be to minimize both error from the modeling effort and financial costs of the observation effort.

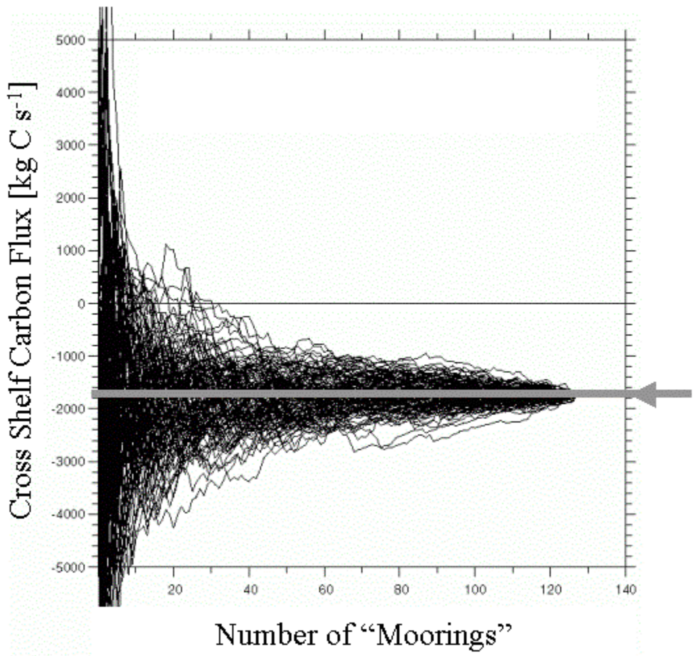

Figure 6. A composite plot of a suite of cross-shelf carbon flux estimates made by randomly choosing an increasing number of grid points “simulated moorings” from a 3D coupled circulation/biogeochemical model (Stolzenbach et al., 2004) to calculate/estimate the flux. As the number of “moorings” increases, the estimate approaches the model solution (thick gray bar with arrow). Of interest to observational oceanographers is the large range and sign changes observed at low (~5)—yet typical—numbers of “moorings.”

Assimilation of ocean color satellite observations into coastal ocean biogeochemical models is still in its infancy. This is partly due to the lack of adequately developed coastal ocean color products. Coastal regions contain a diverse suite of biogeochemical processes, and the bio-optical signature of the allochthonous materials (typically CDOM and sediments) varies in space and time. Because of this, regional algorithms should be developed that use the available higher-resolution (LAC) data sets and Case-II ocean color algorithms that have been optimized or developed for specific coastal regions. Doing so would provide an improved ocean color data set that modeling studies could then use for validation.

All of the model/algorithm applications presented within this chapter have been developed primarily using subjectively defined or chosen algorithms or equations. There are a number of new applied math techniques that will allow for objective development of model equations or algorithms. Several of these (e.g. neural networks, genetic algorithms, fuzzy logic) have been presented in Chapter 9. As these non-subjective techniques become available, new ocean color algorithms and model equations will be developed that are based relationships that have been optimization using data sets. These new techniques will allow for the optimization of both parameters and model equations, thereby removing the subjectivity that now exists in developing model equations.

While open source code development has become popularly supported within the computer software community, it continues to be less accepted within the science community. There is no doubt that open source code development provides an optimized path for creating software applications (e.g. models). It is of benefit to both the science funding agencies and associated scientists to adopt this manner of code/model development. What will be interesting to observe is the path that is taken to develop and support such an effort.

Acknowledgements

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