Ecodynamics and dissolved gas chemistry routines for ocean circulation models

Shaoping Chu\textsuperscript{a,}\textsuperscript{*}, Laurie A. McNair\textsuperscript{b}, Scott Elliott\textsuperscript{b}, Chung-Chieng A. Lai\textsuperscript{b}, Omar A. Hurricane\textsuperscript{c}, Richard P. Turco\textsuperscript{d}, Richard C. Dugdale\textsuperscript{e}

\textsuperscript{a}Institute of Geophysics and Planetary Physics, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
\textsuperscript{b}Earth and Environmental Sciences Division, Atmospheric and Climate Sciences Group, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
\textsuperscript{c}Lawrence Livermore National Laboratory, PO Box 808, L-312, Livermore, CA 94550, USA
\textsuperscript{d}Atmospheric Sciences Department, University of California, Los Angeles, CA 90024, USA
\textsuperscript{e}Romberg Tiburon Center for Environmental Studies, San Francisco State University, PO Box 855, Tiburon, CA 94920, USA

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Abstract

Interactions between oceanic nitrate ecology and circulation determine the marine distribution of dissolved, climate relevant trace gases such as dimethyl sulfide (DMS) and carbonyl sulfide (OCS), and a variety of hydrocarbons. Our group is constructing a suite of ecosystem/reaction/transport models, which link nitrate to the chemistry of volatiles near the sea–air interface. In this paper, we describe programs which will be inserted into the high resolution Parallel Ocean Program. Major features of the coding include: (1) ecodynamics represented in seven biological compartments (phytoplankton, zooplankton, bacteria, detritus, nitrate, ammonium and dissolved organic nitrogen). Light limited primary production is computed, along with nitrogen cycling among the bioentities. (2) Photochemistry for the volatile species DMS, OCS, the methyl halides, nonmethane hydrocarbons (NMHC) and ammonia. DMS and the halides are emitted by phytoplankton, while OCS and NMHC are produced by photolysis of dissolved organic material. Ammonia is exuded by animals and bacteria. Removal mechanisms for the gases include consumption by organisms, hydrolysis, chlorination and interfacial transfer. (3) Explicit, efficient and mass conserving numerical solutions for the biological and chemical continuity equations. Production and loss forms are generalized and automated so that they are readily applied to new constituents. Ecology and the chemical transformations are exposed qualitatively to begin, and are then expressed as differential and differencing equations. The structure of the program is described in terms of the major subroutines and their purposes. Results are provided from both one- and three-dimensional sample runs. Computational aspects such as performance and code availability are discussed. © 1999 Published by Elsevier Science Ltd. All rights reserved.

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1. Introduction

Biogeochemical cycling of nitrogen in the upper ocean, drives several processes crucial to understanding of the earth system. For example, nitrate upwelling
fuels both new and recycled biological production and is balanced by carbon drawdown. Hence, it influences atmospheric carbon exchange (Fuhrman and Capone, 1991; Najjar et al., 1992; Siegenthaler and Sarmiento, 1993). Climate relevant volatiles such as dimethyl sulfide (DMS) are released by marine organisms at rates which depend on those of primary production (Charlson et al., 1987; Fuhrman and Capone, 1991; Andreae and Crutzen, 1997; Watson and Liss, 1998). Because of strong connections between marine ecology and biogeochemistry, ecodynamics programs are under development for insertion into large scale ocean transport simulations (Harrison and Platt, 1986; Fasham et al., 1990, 1993; Doney et al., 1995, 1996). Some are also being coupled to partial photochemical codes representing the transformations of gases in the euphotic zone (McNair et al., 1998). In the present paper, we describe one of the interacting ecodynamical–chemical models. Our code is a hybrid of biology parameterizations from the Fasham group (Fasham et al., 1993; Sarmiento et al., 1993) with programming techniques developed for treating atmospheric photochemistry (Turco et al., 1979; Elliott et al., 1995, 1996).

We begin by describing qualitatively the biophysical systems involved — nitrate driven ecology and the chemistry of related dissolved gases. The volatile species we treat are DMS, carbonyl sulfide (OCS), the methyl halides, nonmethane hydrocarbons (NMHC) and ammonia. They constitute a representative subset of reactive molecules which cross the sea–air interface and influence directly the photochemistry of the atmosphere (Liss and Slater, 1974; Johnson, 1981; Singh et al., 1983; Andreae, 1986; Quinn et al., 1990; Donahue and Prinn, 1992). In the core sections of the text we translate the descriptions into an ordinary differential equation format, and to finite differencing representations which are convenient for solution in the context of ocean tracer transport modeling. Methods are delineated for manipulating a growing reaction list. We ultimately outline the overall structure of the coding which results; the ordering of integration steps is given.

With the model/program detailed the text moves on to offer samples of results. Profiles are provided from one-dimensional simulations of generic open ocean waters. Horizontal sections are shown from an idealized model of a subtropical gyre. The coupling of ecology/chemistry coding into global three-dimensional (3D) tracer transport programs is considered on a preliminary basis, with attention to improvements that will be required. We conclude with a treatment of computational aspects of the problem. Program performance is surveyed over the variety of work station and supercomputer platforms with which we have worked. Information is listed for dissemination of the coding.

2. Nitrogen ecodynamics in the open ocean

Most marine biological activity occurs in the top few hundred meters of the sea, which collectively are known as the euphotic zone because they are sunlit (Sverdrup et al., 1942). Ecology in the upper ocean both tracks and feeds back into climate (Fuhrman and Capone, 1991; IPCC, 1995; Longhurst et al., 1995). Ocean ecosystems and their production depend on physical processes controlling the supply of nutrients to the surface layer. Changes in nutrient input and distributions may influence marine ecosystem structure on large scales. Alterations in new and recycled production are possible and play into the release of radiatively active gases such as DMS, OCS and N₂O (Fuhrman and Capone, 1991; IPCC, 1995; Watson and Liss, 1998).

Nitrogen in the form of nitrate is the nutrient which most often limits plant growth in the sea (Redfield et al., 1963; IPCC, 1995; Mann and Lazier, 1996). It is essential in the synthesis of proteins and other biomolecules. Nitrate is removed from the water column as phytoplanktonic primary producers experience growth. A variety of nitrogen species then cascade into zooplankton and other reservoirs as plants are consumed (Fasham et al., 1990, 1993). N is returned to solution as organisms die and decay. Excretory products are broken down by bacteria and are then reused by new plants and animals (Sverdrup et al., 1942; Duxbury and Duxbury, 1991). Ammonia/ammonium are among the excreta.

A nitrogen-based model developed by Fasham et al. (1990) has successfully simulated euphotic zone ecosystems over a broad range of latitudes (Fasham et al., 1993; Sarmiento et al., 1993). We adopt this work as our conceptual baseline for marine ecology, following it closely to construct representations of the major biological processes. Similar coding from other groups could equally well have been chosen as a foundation. For example, Doney et al. (1995) describe alternate models which capture broad scale features of the major surface ecosystems. We draw on the Doney research for details of vertical mixing and biooptics. Emphasis is placed upon the Fasham approach here mainly for historical reasons. The model we derive has seven compartments: it simulates N transfer between phytoplankton, zooplankton, bacteria, nitrate, ammonium, labile dissolved organic nitrogen compounds (DON), and detritus. The phytoplankton growth rate is attenuated from a maximum value by both light (Harrison and Platt, 1986) and nutrient limitation (Redfield, 1958; Redfield et al., 1963). Nitrate and ammonium are treated as distinct nutrients. Primary production thus divides naturally into new processes fueled by oxidized species, and into a recycled (reduced) portion (Dugdale and Goering, 1967).
Phytoplankton exudation was handled very simply by assuming that a constant fraction (5%) of photosynthesis was expelled as DON.

The model zooplankton feed on phytoplankton, detritus, or bacteria. The fraction of each food type that is consumed must be specified. Fasham et al. (1990) developed an algorithm in which preference for a particular source depends on its relative concentration. Three fourths of ingestion are assimilated, while one-fourth is discarded immediately. The discard is assumed to consist of fecal pellets. Excretion is described as a linear function of zooplankton mass. Nitrogen lost is distributed, 75% as ammonium and 25% as DON. Animal mortality is also modeled as a function of biomass. Two-thirds of dead material are distributed to the ammonium bin and one-third to detritus. The detrital reservoir is the sum of dead phytoplankton mass and zooplankton fecal pellets. Detritus was assumed to move through the euphotic zone with a constant sinking rate of 10 m/day, an optimum determined by Fasham et al. (1990) through sensitivity tests in a model spanning the North Atlantic basin.

3. Some gas chemistry in the open ocean

Several volatile compounds produced either directly or indirectly by marine organisms enter into photochemical cycles within the water column and later influence atmospheric processes (Fuhrman and Capone, 1991; IPCC, 1995; Watson and Liss, 1998). We provide here a selective review of species falling into this category and incorporated into our model. In some cases, the importance of an individual molecule within the earth system renders its consideration unavoidable. Other species we deal with are related by chemical structure or along a kinetic decay sequence. Many of the reactions cited have been studied as part of our laboratory work (Elliott et al., 1987,1989; Elliott and Rowland, 1993,1995). Major production and removal processes are listed for addition to the nitrogen ecodynamics. Some useful encompassing reviews of the subject are contained in the monograph by Buat-Ménard (1986). These, however, are now old enough that they must be viewed as foundation literature. More recent references include the 1995 IPCC report chapter on marine ecology and Ratte et al. (1993), Andreae and Crutzen (1997), or Watson and Liss (1998).

Dimethyl sulfide (DMS) is the predominant volatile sulfur compound in the open ocean and the major natural source of sulfur to the atmosphere (Andreae and Crutzen, 1997). When ventilated from the sea, the molecule is oxidized to produce aerosol particles which may affect the radiative properties of marine stratus clouds (Twomey, 1974; Charlson et al., 1987). Early conceptions of the overall marine DMS cycle were overly simple; it was thought that production was proportional to phytoplankton biomass, and that removal consisted of consumption by bacteria, or transfer upward or downward out of the euphotic zone (Andreae, 1986). Several new pathways are now attached to most models and include sources of DMS due to senescence and grazing (Gabric et al., 1993; Malin et al., 1993).

Carbonyl sulfide (OCS) is the most abundant sulfur species in the remote troposphere. Due to its low reactivity with hydroxyl radical and the correspondingly long gas phase residence time, it is the primary sulfur compound that enters the stratosphere. There it is the major source of sulfur atoms to the Junge aerosol layer (Andreae and Crutzen, 1997). In the upper part of the ocean, OCS is produced by photochemical reactions from dissolved organics (Andreae, 1986) and then hydrolyzed rapidly (Johnston, 1981; Elliott et al., 1987), resulting in strong diurnal cycles. Ventilation into the atmosphere and mixing downward into the deep ocean are other loss modes (Johnson and Harrison, 1986; Weiss et al., 1995). The hydrolysis takes place through the reaction of either the water molecule itself or the hydroxide ion with species in the carbonate analog acid–base system (the monothiocarbonates; Elliott et al., 1989). At the oceanic pH of 8 and average surface temperatures, the time constant is several hours. Since this is faster than mixing to the surface, most OCS is processed in the water column. The family of hydrogen sulfides (H₂S, SH⁻, S₂⁻) is the product of OCS hydrolysis. Their alternate sources and oxidation rates are highly uncertain. We plan to include them as more information becomes available.

The oceanic methyl halides constitute the largest natural source of halogen atoms to the stratosphere, being surpassed of course with the advent of chlorofluorocarbon manufacture (Rowland and Molina, 1975; Singh et al., 1983). The sea has recently been under scrutiny for its role in the atmospheric methyl bromide budget (Lobert et al., 1995; Pilinis et al., 1996). Methyl iodide transports iodine atoms to the upper troposphere, where they impact ozone production (Davis et al., 1996). The marine chemistry of the halides is strongly interlocking. Methyl chloride (CH₃Cl) is produced by phytoplankton (Singh et al., 1983; Liss, 1986) and by chlorination of methyl bromide (CH₃Br) and methyl iodide (CH₃I) (Elliott and Rowland, 1993). It is removed abiotically, through hydrolysis (Elliott and Rowland, 1995). Transfer across the air/sea interface and downward mixing into deep ocean must also be considered. The chemistries of methyl bromide and iodide are similar, and chlorination is a significant loss channel. Both species are also produced by marine plants (Liss, 1986). Recent studies show that methyl bromide is also removed biologically, by bacteria (King and Saltzman, 1997). Rates
are as yet poorly defined but the loss constant for the open ocean appears to be about 10 days. Bacterial consumption may extend to other organohalogenes. The methyl halide chlorination–hydrolysis sequence leads finally to methanol, which is thermodynamically stable in the water column. It vents from the sea and contributes to gas phase alcohol chemistry (Singh et al., 1983; Elliott, 1984).

The nonmethane hydrocarbons (NMHCs) act in the troposphere as sources and sinks for ozone (Liu et al., 1987; Crutzen, 1988; Singh and Zimmerman, 1992). Alkane oxidation is initiated by the hydroxyl radical. Unsaturated species may react with ozone as well. Organic decomposition leads to a net splitting of the O2 bond, if the nitrogen oxides are available for catalysis (Elliott et al., 1995, 1996). The ocean is a source for many of the nonmethane species (Donahue and Prinn, 1992; Ratte et al., 1993). NMHCs are generated in the surface sea from dissolved organic material (DOM) through little known photolytic mechanisms (Ratte et al., 1993; Broadgate et al., 1997). Downward mixing and ventilation are again crucial loss pathways. Most light alkanes and alkenes are supersaturated in the waters of the North Atlantic (Ratte et al., 1998). Acetylene is an exception, being present at near Henry’s law equilibrium. Ethylene concentrations tend to be highest, followed by those of propylene. It can be demonstrated in the laboratory that dissolved organics are the dominant source of NMHCs; simulants added to water samples photolyze to give the same organic molecules detected in the sea. Quantum yields as functions of wavelength are beginning to be tabulated. In our routines, photosynthetic radiation is not resolved spectrally (Fasham et al., 1993; Sarmiento et al., 1995).

Acid–base interactions play a significant role in chemistry of the remote marine troposphere (Junge, 1963; Stumm and Morgan, 1970; Quinn et al., 1990; Pilinis et al., 1995). The primary base is ammonia. It exists in five phases in the marine environment: as the atmospheric gas NH3, in the aerosol phase as ammonium ion NH4+, in rain and cloud water as NH2+, and in sea water in both the ionized and unionized forms (Quinn et al., 1990). In our model, ammonia is handled as both a nutrient and an interface-crossing volatile. It is excreted by zooplankton and bacteria into sea water. The bulk of the reduced nitrogen is then available to drive plant growth, while the volatile fraction is permitted to flux from the surface. DMS oxidation produces the sulfuric acid which is thought to neutralize ammonia within the particles and hydrometeors of the oceanic regime (Quinn et al., 1990). DMS release is associated with phytoplanktonic activities, while NH3/NH4+ is injected into the water column by bacterial and animal metabolics further along the ecodynamical cascade of nitrogen atoms. Sea–air transfer of NH3 may, thus, be phase lagged relative to that of DMS. This possibility has implications for the seasonality of aerosol and cloud pH. The equilibrium NH3 + H+ \rightleftharpoons NH4+ is considered here to be established instantaneously (Stumm and Morgan, 1970), but is computed only in the surface layer. The NH3 fraction alone is transferred into the gas phase. The ammonia–ammonium couple is transported collectively elsewhere. It functions as a nutrient in all layers.

4. Governing equations

In this section, we cast the ecodynamics and ocean chemistry into mathematical form. Our main interest is in processing internal to water parcels. Hence, we move rapidly from partial to ordinary differential equations. Specific terminology follows the presentation of Sarmiento et al. (1993), an early effort to insert nitrogen cycling into the ocean tracer transport context. Their approach is maintained as biological expressions are constructed, then is extended to encompass the chemical transformations of the gases. Addition of the abiotics roughly doubles the number of tracers and of ode’s. Our manipulations, thus, also reflect experience with the stiff ordinary differential equations encountered in atmospheric chemistry/aerosol models (Turco et al., 1979; Elliott et al., 1995, 1996). Overall, the derivation is patterned after developments presented by Elliott et al. (1993, 1996) for tropospheric photochemistry.

The coupling of transport and intracellular processes is dealt with first, in Eqs. (1)–(9). Ecology and then chemistry are appended, as sets of ordinary differentials. We provide only a sketch of the full set of equations. Where more biological detail is desired, the reader may refer to (Fasham et al., 1990) and (Fasham et al., 1993). These authors and the Doney group (Doney et al., 1995, 1996) summarize preferred values for nitrogen ecology rate parameters. The equations governing chemistry of the gases are expanded from the concepts presented in (McNair et al., 1998). Unless otherwise stated, all quantities are manipulated in units of millimoles nitrogen m−3. This is equivalent to micromolar, a standard unit in chemical oceanography (Broecker, 1974; Broecker and Peng, 1982).

Volatiles not containing nitrogen are tracked as concentrations of the molecules themselves. For single carbon species this is in fact an accounting of C atoms.

Continuity for individual nitrogen containing species or the gases they produce takes the general form

\[
\frac{\partial C}{\partial t} = -\nabla \cdot \Phi + \text{PML}(C),
\]

with PML(C) = p(C) − l(C), where \( \Phi \) is a flux, and \( C \) is
the vector of concentrations corresponding to the system components. The biological and chemical terms are indicated by PML, an informal abbreviation for production minus loss. We use the symbols PML and \( p - l \) interchangeably. In some cases, it is numerically expedient to treat positive and negative terms separately (Elliott et al., 1993, 1995, 1996). The flux consists of advective components \( uC \), where \( u \) is the velocity field, as well as diffusion terms. Time splitting is used to separate chemistry and transport numerically (Yanenko, 1971; McRae et al., 1982a,b; Rood, 1987). Eq. (1) can be transformed to the sequential operators

\[
\frac{\partial C}{\partial t} = -\nabla \cdot \Phi,
\]  

(2)

\[
\frac{dC}{dt} = \rho(C) - J(C).
\]  

(3)

To represent situations within which multiple species interact, the above equations are converted to scalar subscripted formats.

\[
\frac{\partial C_i}{\partial t} = -\nabla \cdot \Phi(C_i),
\]  

(4)

\[
\frac{dC_i}{dt} = p_i(C_i) - l_i(C_i).
\]  

(5)

in which subscripts \( i \) and \( j \) can vary over all constituents, or

\[
\frac{dC_k}{dt} = f_k(C)
\]  

(6)

in which subscript \( k \) can vary over constituents alone or over constituents and the grid; the full vector statement

\[
\frac{dC}{dt} = f(C)
\]  

(7)

is equivalent to (6).

Finite difference relationships are also readily transposed to vector notation; for example, the forward (explicit) and reverse (implicit) Euler solutions of (7) become, respectively,

\[
C^{t+1} = C^t + \Delta t f(C^t)
\]  

(8)

\[
C^{t+1} = C^t + \Delta t f(C^{t+1})
\]  

(9)

We rely primarily on explicit solutions to our ecochemistry because they are straight forward, mass conserving and stable under the conditions of interest. The time step in the codes we have applied varies from 1.5 to 2 h. Since this is less than a photoperiod, diurnal cycling is adequately represented. If negative concentrations appear, we superimpose mass conserving implicit solutions within the problem cells. The process is needed only rarely and is described in (Elliott et al., 1993, 1995, 1996). The coupled ecochemistry system remains relatively simple for the moment. A quick inspection of time constants is still sufficient to demonstrate that for most constituents and at most times, forward differencing will not destabilize. This situation is to be contrasted with the state of the art in atmospheric photochemical simulations. Hundreds of reactions may be tracked (e.g., Atkinson and Lloyd, 1984; Liu et al., 1987; Demore et al., 1990; Donahue and Prinn, 1992; Elliott et al., 1995, 1996), and often in three dimensions (e.g., McRae et al., 1982a,b; Trainer et al., 1987; Crutzen and Zimmermann, 1991; Jacob et al., 1993a,b). Local species lifetimes vary upward from nanoseconds (Brasseur and Solomon, 1984).

It is expected that detailed oceanic radical photochemistry will someday be attached to codes such as ours (Zafiriou et al., 1984; Plane et al., 1997). The level of complexity will then approach or surpass that attained in the atmosphere.

The explicit forms of the solutions are rapidly advanced on most computer platforms because the individual species versions can be solved independently of one another. In equations such as (9) or the related linear multistep backward differentiation formulae (Gear, 1971; Byrne and Hindmarsh, 1987), coupled systems require iterative techniques such as the dimensional Newton Raphson (Hornbeck, 1975). The intermediate strategy of local linearization may be non-conservative (Elliott et al., 1995, 1996). Our calculations are set up in anticipation of vector or parallel processing capabilities by placing geographic do loops inner most (Elliott et al., 1993, 1995; Jacobson, 1995, 1998; Jacobson et al., 1996). In large scale environmental models, the maximum for indices of physical length exceed the number of vector registers or of distributed processors, which optimizes performance (Metcalff, 1982; Levesque and Williamson, 1989). Global ocean circulation models now attain resolutions approaching one-tenth degree in longitude and latitude (Smith et al., 1992; Dukowicz et al., 1993; Dukowicz and Smith, 1994). Even in one of the horizontal dimensions the number of cells may be many hundreds. In the time split mode of operation Eqs. (3) and (5) can be solved on a single index, sequencing the geographical dimensions (Elliott et al., 1993). The parallel length becomes virtually unlimited.

The ecosystem model is solved for the upper 100 m or so of our model oceans. Biological interaction terms defined by Eqs. (10a)–(10g) below (Sarmiento et al., 1993):

\[
PML(P) = (1 - f_1)J(z,t)(Q_1 + Q_2)P - G_1 - m_1 P
\]  

(10a)
\[ PML(Z) = f_2(G_1 + G_2 + G_3) - (m_2 + m_3)Z \]  
\[ PML(B) = U_1 + U_2 - G_2 - m_1B \]  
\[ PML(N_a) = -j(z,t)Q_1P \]  
\[ PML(N_a) = \left[ f_1m_2 + (1-f_2)m_3 \right]Z + m_1B - \]  
\[ + \frac{G_2 - m_4N_a - w_s \frac{\partial N_a}{\partial z}}{10b} \]  
\[ PML(N_d) = m_1P + (1-f_3)(G_1 + G_2 + G_3) \]  
where \( P \) represents phytoplankton, \( Z \) zooplankton, \( B \) bacteria, \( N_a \) nitrogen as nitrate, \( N_o \) nitrogen as ammonium, \( N_d \) dissolved organic nitrogen and \( N_z \) nonliving particulate organic nitrogen. The subscripts 'n' and 'a' refer to the two main channels of primary production — new and recycled (Dugdale and Goering, 1967). Capital \( J \) indicates a light limitation, \( Q \) a nutrient or resource limitation, \( G \) a grazing term and \( U \) a bacterial uptake term. The coefficients \( f \) are attached to fractions of processes and have values between 0 and 1 (dimensionless). The \( m \) are time constants for mortality, which have units of \( d^{-1} \). The \( w_s \) is a detrital sinking velocity. The quantities \( Q \) resemble Michaelis–Menten enzyme kinetics expressions and are fully delineated in (Fasham et al., 1990; Sarmiento et al., 1993). Nitrogen nutrient thresholds are incorporated. A general form is \( Q = N/(K + N) \) where \( K \) is a half saturation value in the usual units. The grazing terms include food preference and switching information. Proportionalities to local resource concentrations are embedded. The threshold concept again applies but the variety of food items become the nutrients.

Zooplankton consume phytoplankton, bacteria and particulates (\( P, B, N_a \), correspond to 1, 2 and 3). In the parlance of Eqs. (4) and (5), much of the variation over \( j \neq i \) occurs in the \( Q \) and \( G \).

Light limitation is contained in the \( J \) parameter for plant growth.

\[ J(z,t) = zI(z,t) \quad \text{or} \quad V_p \]  
where \( z \) is the initial slope of the photosynthesis versus irradiance (\( P-I \)) curve in \( d^{-1} \) (\( W \ m^{-2} \)). \( I \) is irradiance in \( W \ m^{-2} \), and \( V_p \) is the growth rate in \( d^{-1} \) as \( I \rightarrow \infty \). The \( V_p \) value is taken from (Harrison and Platt, 1986). \( V_p = 0.6(1.066)^t \) is their empirical relation and light attenuation is expressed as

\[ I(z,t) = I(t)_{z=0} \exp \left( -k_a z - \int_0^z k_d P dz \right) \]  

The Beer’s law fall off is determined by coefficients for absorption/scattering by the water medium (\( k_a \) and plankton (\( k_d \)). The variable \( P \) is defined in 10. Irradiance just below the surface of the ocean \( R(t)_{z=0} \) is calculated using a clear sky value with diurnally varying solar angle (Brasseur and Solomon, 1984), then adjusting for (1) the portion of the radiation that is photosynthetically active, (2) the effect of cloud cover (NCAR Technical Report, 1982; Peixoto and Oort, 1992; Sarmiento et al., 1993), and (3) refraction.

Transformation of the volatiles involves release and uptake by biological entities, along with aqueous phase chemistry. A distinct chemical-type kinetics applies to the gases. The threshold forms are less relevant. Removal processes are represented either as liquid phase unimolecular or bimolecular reactions. We have added PML for the gases: DMS, OCS, CH₃Cl, CH₃Br, CH₄, the hydrolysis product methanol and NMHC. We signify the species and their concentrations as \( V \) for volatiles, and number them from one to seven. Dissolved ammonia gas concentrations (\( V_6 \)) are computed from the ecodynamics through standard acid/base equilibria. The transformation mechanisms are

\[ PML(V_1) = k_{p1}P - k_{l1}BV_1 \]  
\[ PML(V_2) = k_{p2}I(z,t)N_a - k_{l2h}V_2 \]  
\[ PML(V_3) = k_{p3}P + k_{hb}Cl^-V_4 + k_{j1}Cl^-V_5 \]  
\[ - k_{l3h}V_3 \]  
\[ PML(V_4) = k_{p4}P - k_{hb}Cl^-V_4 - k_{l4h}V_4 \]  
\[ - k_{l4}BV_4 \]  
\[ PML(V_5) = k_{p5}P - k_{j1}Cl^-V_5 - k_{l5h}V_5 \]  
\[ PML(V_6) = k_{l3h}V_3 + k_{l4h}V_4 + k_{l5h}V_5 \]  
\[ PML(V_7) = k_{pe}I(z,t)N_o \]  
\[ k_{pe} \text{ and } k_{l pe} \] are production and loss coefficients, respectively, for the volatiles. As a rule, loss rates are known from laboratory studies (e.g., Elliott et al., 1989; Elliott and Rowland, 1993,1995; King and Saltzman, 1997), but production must be determined through iterative model runs and comparison with field measurements. Subscript 'h' points to hydrolytic
processing, whether for OCS or the halides. The average Cl– concentration is set to 0.5 molar. While the ecoquantities are confined to the water column, all the volatiles we discuss transfer from ocean to atmosphere.

The process is often parameterized through a double laminar layer interface model. Flux matching ($F$) allows the elimination of unknowns at the sea surface. We have relied upon the formulation of Liss and Slater (1974). For the majority of gases, transfer is rate limited in the liquid phase:

$$F = K_w(C_w - C_a)H^{-1}$$  \hspace{1cm} (14)

For some soluble gases such as ammonia and methanol, transfer is subject to gas phase limitation,

$$F = K_g(HC_w - C_a)$$  \hspace{1cm} (15)

In Eqs. (14) and (15), $C_w$ and $C_a$ are the gas concentrations in air and water in units of mmol m$^{-3}$, respectively, $K_w$ and $K_g$ are the sea–air exchange constant in units of m d$^{-1}$. $H$ is the dimensionless Henry’s law constant (expressed as the ratio of the concentration of gas in air to its concentration in unionized form dissolved in the water, at equilibrium). Broecker and Peng (1982) presented closely related forms. Early authors derived only global average values for the piston velocity $K_w$ (typical values were 0.2 m h$^{-1}$). It can now be expressed as a function of wind speed (Wanninkhof, 1992). Other refinements are listed in references, such as Liss (1986) and Liss and Merlivat (1986).

The equation sets (10a)-(10g) and (13a)-(13g) are both likely to become larger in the near future. It is clear that global scale marine ecology is only crudely simulated in the handful of ecocompartments we adopt. Dozens of biomes can be identified across the oceans of the world, as functions of latitude and circulation (Sverdrup et al., 1942; Longhurst et al., 1995; Mann and Lazier, 1996). Even if the aggregated species in Eqs. (10a)-(10g) are retained, rate parameters will vary geographically. New species will be needed as well. Super predators can be conceived lying above zooplankton in the trophic structure. The phytoplankton should be resolved taxonomically and with respect to size structure (Fasham et al., 1990,1993; Doney et al., 1995). Additional nutrient species will be needed, also. Specifically, the inclusion of silicate as a potentially limiting nutrient will be necessary as diatoms are added to the primary producer level. (Dugdale et al., 1995; Dugdale and Wilkerson, 1998). As size binning within living or detrital ecocompartments is implemented, analogies with aerosol microphysics of the atmosphere will become more apparent (Turco et al., 1979; Brun-Cottan, 1986; Pandis et al., 1995). We have mentioned that product species such as the hydrogen sulfides could yet be appended to Eqs. (13a)-(13g), along with their oxidation products and an overall radical photochemistry (Zafiriou et al., 1984; Elliott et al., 1987).

Programming for additional species/reactions will become increasingly difficult as Eqs. (10a)-(10g) and (13a)-(13g) grow. The effort required scales more than linearly because of new linkages between constituents. We have encountered a similar problem over the last two decades in our studies of chemistry of the atmosphere. Automation of the set up of solutions has proven an effective strategy (Elliott et al., 1995,1996). New processes are readily inserted. Sensitivity testing is facilitated. Our ecochemistry programs extend the concepts to include the forms in the biological continuity equations. The following paragraphs provide a flavor for the level of coding complexity entailed.

Mass conservation is assured in our model by cross cancellations in the equations and reliance on explicit numerics. Relative to (10a)-(10g) and (13a)-(13g), continuity expressions for nitrogen, sulfur, chlorine or carbon atoms contain fewer entries—in fact, only those which connect the atomic systems or exit atoms from the set of compartments under consideration. Individually the (10a)-(10g)/(13a)-(13g) terms represent rates for processes transferring atoms among the bins. By the laws of population ecology, nutrient ecology and chemical kinetics, the single rates often take the general form (Brasseur and Solomon, 1984; Edelstein-Keshet, 1988; Mann and Lazier, 1996)

$$R_{IR} = k_{IR} \Pi_j(C^*_j)\alpha_j (C_j + K_{j,IR})^{\beta_j}$$  \hspace{1cm} (16)

where $j$ varies over species, and $IR$ is a process index defined for programming purposes. The proportionality $k$ is a rate/growth constant. Capital $K$ are resource thresholds. The power constants $\alpha$ and $\beta$ take the values $-1, 0$ or $1$, and so serve as switches for species contributions.

Data input lists of the coefficients and species involved in Eq. (16) are readily initiated or altered. Information may appear as lines or cards with the columns

$$IR, k, j, x, \beta, K, j, x, \beta, K, \ldots$$  \hspace{1cm} (17)

These constitute coefficient vectors. They can also be tabulated in rows referring to species; Eq. (17) has conceptual advantages. Locations within the ordinary differentials can be similarly organized.

$$IR, d, j, \delta, \ldots$$  \hspace{1cm} (18)

where $\delta$ now indicates production, loss or nonparticipation. Nonspecified values default to zero as a space and time saving device in both sets. With respect to the chemical kinetics, Eqs. (17) and (18) correspond...
closely to stoichiometries and the conventional reaction equation

$$\sum \gamma_{j} C_{j} \rightarrow \text{products} \quad (19)$$

In fact, in our atmospheric programs, we have traditionally tabulated rate parameter data in such arrays. Vectors of temperature/pressure dependencies are included. Checks for mass consistency may be automated into the system as well. The ecological growth and Michaelis–Menten mechanisms are more difficult to relate to elementary steps (Edelstein-Keshet, 1988). We offer no biological analog for Eq. (19).

Explicit (Eq. (8)) rate contributions from the IR to $C^{i+1}$ can be constructed from Eqs. (16)–(18) with $C_{j}$ lifted from the model grid. Geography is looped inside not only to ensure that parallel lengths are exceeded, but also to avoid recursion. The collapsing of (16) into PML constitutes an array to scalar operation and is, thus, necessarily inhibitory (Levesque and Williamson, 1989; Elliott et al., 1993). For implicit versions of our finite differencing Eq. (9), it is coefficients for linearization that are built up. The technique is analogous to our descriptions here, but is more challenging to program (Jacobson, 1995,1998; Jacobson et al., 1996). The automation methods can even accommodate partitioning of species grouped together as rapidly interchanging families (Brasseur and Solomon, 1984; Elliott et al., 1993,1995,1996). This feature has not yet been applied in our ocean ecochemistry models but could become necessary at some point. Currently, our only family group is the NH$_{3}$/NH$_{3}$ couple, which we handle off-line.

The biology on occasion requires special adjustments to the rate formula in Eq. (16). For example, Fasham et al. (1990,1993) damp nitrate uptake in the presence of ammonia because reduced N is more easily assimilated and so is preferred. The attenuation is expressed as an exponential in the NH$_{3}$ concentration. Our programming treats the special cases in separate routines.

5. Code structure

The automation setup requires only a single call, and so is placed/run at the top of the code sequence. Because the coefficient vectors are read only once, there is little effect on computational performance. This is the case despite considerable programming complexity (Elliott et al., 1993; Jacobson, 1995; Jacobson et al., 1996). Logical ‘if’ statements abound as the constituent and reaction terms are sorted for processing. Fixed (nonspecies and nonreaction dependent) process parameters are read in alongside the vectors. Examples include the water column and phytoplanktonic light extinctions. They as yet contain no wavelength dependence, although spectral information may soon be needed to couple with emerging data on absorption cross-sections for NMHC production.

Next, a set of arrays are input which represent physical properties of the ocean distributed over the grid, as function of time. Local temperature and vertical eddy diffusivity are the most important quantities. We have available both empirical, measurement based data sets and values derived from ocean general calculation model runs. Our primary OGCM resource is the Bryan Cox Semtner family of programs (Bryan, 1969,1989; Semtner, 1986; Smith et al., 1992). Eddy diffusion may be computed in either a direct Richardson number-based approach (Pacanowski and Philander, 1981) or through the Large et al. (1994) k-profile parameterization (KPP) scheme. In some versions of the ocean circulation simulations, sea surface temperatures are restored to climatological values at the surface so that our modeled quantities are indirectly empirical. The empirical data bases drawn upon are: (1) for temperature Levitus (1982) and similar atlas materials, and (2) for diffusion collections of observations and model results (e.g., Sverdrup, 1942; Riley and Skirrow, 1975; Li et al., 1984; Parker, 1991; Doney et al., 1995).

Starting concentrations are now spread over the physical mesh, for the biological and chemical tracers. For organisms we initialize at roughly an order of magnitude below minimum open ocean surface values. We determine the starting points through a survey of measurements and models (Fasham et al., 1993; Gurney et al., 1993; Mann and Lazier, 1996; Longhurst et al., 1995), then iterate downward where guesses have been too high (where populations fall rather than rise toward steady state). The organismal growth kinetics are often first order. Reasonable base-lines are required so that the overall biological equilibrium can be approached within upper ocean mixing time scales.

Clock variables are set just above the main integration loop. A time manager tracks the numbers of seconds, hours, days and months which have elapsed and passes consistent information to all routines. The subprograms derive from diverse sources around the earth system community; the task of dimensional conversion is not entirely trivial. Our runs are generally one season to several years in length. Midlatitude phytoplanktonic blooms can be studied numerically over just a few months. A steady annual biological cycle is attained at the basin scale only over three to five years (Sarmiento et al., 1993). The time step is adjustable in our programs. However, a step size of one to three hours has generally been used. We seek to avoid diurnal averaging of light penetration by resolving the
photoperiod. In part, this is because we anticipate a rich photochemistry. Simultaneously, computational efficiency is desired. Our choice of $\Delta t$ represents a compromise between these and other factors. While Sarmiento et al. (1993) have conducted successful basin scale simulations of nitrogen ecodynamics under diurnally averaged conditions, Doney et al. (1995, 1996) stress rapid variation of light and mixing parameters in the upper ocean. Our feeling is that discrimination of the major daily photon and energy cycles will be crucial in the next generation of euphotic zone chemistry models.

As the integration begins, solar and attenuation routines are called upon. Local sunrise, sunset and solar angle are computed in subprograms normally used for tropospheric photochemistry simulations (Elliott et al., 1995, 1996). The standard ephemeris is incorporated (Brasseur and Solomon, 1984). Attenuation of incoming radiation by absorption and cloud/aerosol scattering is parameterized. At the sea surface a refraction correction is applied (Sarmiento et al., 1993). Absorption by phytoplankton and particles in the water column are computed in a discretized version of Eq. (12).

Fig. 1. Concentration contours on a depth versus time grid, from a one-dimensional model of nitrogen ecodynamics representing a subtropical gyre center, 30° North latitude. Units are mmol m$^{-3}$ of nitrogen atoms. Top — nitrate; bottom — phytoplankton.
For most of our runs, transport algorithms are applied just prior to the detailed ecochemistry integrations. In the models described here, the motions represented are either vertical and purely diffusive, or are three-dimensional. The transport operator could also be inserted after solution of local, time split ODEs (Yanenko, 1971; McRae et al., 1982a,b). The effect of altering its position is relatively easy to test because calling statements can simply be edited within the driver program. We have not formally analyzed the results of permutations in the order of our time split operators. The ecology and chemistry are advanced at the end of the main code sequence. The reaction and species rate parameter coefficients are computed based on local temperature and light conditions. Rates are constructed for each process, then are collapsed selectively into PML (production minus loss). Delta concentrations are calculated and all local values are augmented. Loops over geography are prioritized because in 3D models the indices of the physical directions are long. Recall also that the summation of rates into production and loss terms is a recursive, array to scalar function (Levesque and Williamson, 1989; Elliott et al., 1993).

6. Sample calculations

The preliminary one-dimensional ecodynamics model is designed to represent biogeochemical properties of the water column at latitude 30° north, near an oligotrophic gyre center. The upper boundary condition is closed for the ecocompartments. Gases are permitted to transfer across the air–sea interface (Liss and Slater, 1974). At the bottom, boundary nitrate concentration is fixed at thermocline values. The Northern Hemisphere gyres are large in area and often studied. Both measurement and model data are available for comparisons (Fasham et al., 1993; Gurney et al., 1993; Longhurst et al., 1995; Doney et al., 1995, 1996). Our simulations closely reproduce the upward transport of nutrient nitrogen in the winter, and also the spring phytoplanktonic bloom. Depth-time contours of modeled nitrate and phytoplankton densities are displayed in Fig. 1.

From among the climate relevant volatiles, DMS, OCS, the methyl halides and generalized NMHC have all been incorporated into the one-dimensional ecosystem model. Cycling mechanisms in the code are the ones summarized in Eqs. (13a)–(13g). DMS is produced at a constant release rate from phytoplankton. The rate is set arbitrarily initially, then adjusted to give concentrations agreeing with open ocean measurements (Andreae, 1986; Bates et al., 1987; Quinn et al., 1990; Kiene and Bates, 1990). Removal is proportional to bacterial densities and is given a time constant of three days. These simple DMS pathways are based primarily on the early work by Andreae (1986). They should be sufficient for demonstration of the code and to achieve a general understanding of distributions. In future, we will partition release into direct algal emissions and cell lysis pathways, and involve the intermediates dimethyl sulfoxide and dimethyl sulfonium propionate (Gabric et al., 1993). We will also consider taxonomic variation in release mechanisms. Time dependent DMS concentration patterns in the one-dimensional model are similar to those of the phytoplankton because they constitute the major source.

Fig. 2. Carbonyl sulfide diurnal cycling in the Fig. 1 model, for an eight day period in the summer. Units of concentration are mmol m⁻³.
Distributions for the methyl halide group (CH₃Cl, CH₃Br, CH₃I) also parallel phytoplanktonic densities. The major removal for the bromide and iodide is chlorination, which yields methyl chloride (Elliott and Rowland, 1993).

To form a conceptual bridge to full 3D tracer transport calculations, it was felt desirable to perform pedagogical level runs in an idealized model of basin scale flow. In the middle nineteen forties, the American oceanographer Stommel (1948) developed an analytical solution for the stream function across a North Pacific-like subtropical gyre. The solution was based on mixed layer depth averaging. The balance of pressure gradient, coriolis and frictional boundary forces was computed within the standard equations for horizontal motion. A special feature not incorporated into earlier analytical models of gyre flow was the inclusion of latitudinal variation for the coriolis force. This led to an intensification of the western boundary current which closely approximated the situation in the real ocean. Hecht et al. (1995) have used the Stommel stream functions to obtain a self-consistent velocity field for tests of oceanic advection schemes. We have followed Hecht's lead by creating a simple, 3D model which we intend to use for illustrative purposes. We have coupled 10 m layers via eddy diffusion, and

Fig. 3. Surface phytoplankton concentration contours in an idealized model of North Pacific subtropical gyre flow coupled to the one-dimensional ecochemistry routines. Units are mmol m⁻³ nitrogen atoms. Top — April; bottom — September.
advect within each of them using the Stommel velocities and the MPDATA scheme ultimately recommended by Hecht.

The one-dimensional ecoprogram was moved into the idealized basin flow to simulate coupling of ecology and transport. Lower nutrient boundary concentrations were set at the values mapped in Levitus et al. (1993). Figs. 3–6 show phytoplankton, DMS, CH₃Cl and propylene concentrations (mmol m⁻³) in the idealized basin circulation model in April and September. Results are given only for the surface layer. For phytoplankton the low productivity of the equatorial regions, the spring bloom at mid latitudes, and the northward bloom migration are all represented (Fig. 3; Fasham et al., 1993; Sarmiento et al., 1993; Longhurst et al., 1995). Superimposed over these banded structures are the effects of the rapid movement northward in the intensified western boundary current. The advected ecosystems consist of a mixture of low latitude, low productivity and mid latitude waters. In the wide, slow return flow on the eastern side of the idealized Pacific Basin, the ecodynamics enter into relatively rapid, local steady states. In the eastern currents, the time constant for transport any significant distance is years. For DMS, time dependent concentration patterns are similar to those of phytoplankton because
they constitute the major source (Fig. 4). Parallels with
the phytoplanktonic densities are again apparent in
methyl chloride distributions (Fig. 5). Note that signifi-
cant storage occurs late in the year at high latitudes.
In cold northern waters chemical removal is slow.
Propylene is selected as a representative of the
NMHC. Overall patterns are strongly influenced by
phytoplankton (Fig. 6). In April, however, hydro-
carbon and phytoplankton contours are mirror images
in the subtropics. This is probably due to the attenu-
ation by phytoplankton of radiation, and so also of
photolytic production.

The Stommel type advection coupled to the Fasham
ecodynamics has proven to be an extremely useful tool
for visualizing and interpreting the interactions
between ecology and chemistry/transport in the surface
ocean. Many of the major features of real North
Atlantic and Pacific biology were simulated and so
could be clearly understood (Fasham et al., 1993;
Sarmiento et al., 1993; Longhurst et al., 1995). We
envision sensitivity tests within the Stommel program,
regarding the overall distribution of the ecocompart-
ments, and the gases they produce which are of interest
to atmospheric chemists (Andreae, 1986; Liss, 1986;

Fig. 5. Surface methyl chloride concentration contours in an idealized model of North Pacific subtropical gyre flow coupled to the
one-dimensional ecochemistry routines. Units are mmol m$^{-3}$ nitrogen atoms. Top — April; bottom — September.
Charlson et al., 1987; Ratte et al., 1993; Lobert et al., 1995; Weiss et al., 1995; Andreae and Crutzen, 1997). The code is easy to alter and computationally efficient, and so may be an appropriate vehicle for preliminary investigations.

Our ultimate goal is to add the ecodynamics and dissolved gas routines to a large scale circulation model—the Los Alamos National Laboratory Parallel Ocean Program (POP; Smith et al., 1992; Dukowicz et al., 1993; Dukowicz and Smith, 1994). The mesoscale eddies which constitute oceanic weather systems are roughly 100 km in horizontal extent, requiring resolution on the order of one-tenth of a degree globally to avoid parameterization (Bryan et al., 1998). The massively parallel processing machines at Los Alamos have been used to promote the Geophysical Fluid Dynamics Laboratory family of ocean circulation programs (Semtner, 1986; Sarmiento et al., 1993) to the ultrahigh resolutions (Smith et al., 1992). Time constants for many of the eco/chemical processes are similar to those in mesoscale ocean eddies. Horizontal turbulence is, thus, likely to be crucial in determining interplay of ecology and volatile chemistry in the euphotic zone. POP will make it possible to perform global scale simulations/visualizations of ecodynamics and biogeochemical processes in surface waters.

Fig. 6. Surface propylene concentration contours in an idealized model of North Pacific subtropical gyre flow coupled to the one-dimensional ecochemistry routines. Units are mmol m⁻³ nitrogen atoms. Top — April; bottom — September.
Fig. 7. An inert aeolian pollutant is deposited on the Pacific surface daily for four years and advected, in the 2/3° POP. Concentration units are arbitrary. Axis labels are horizontal grid cell numbers. Top — 2 months; bottom — 4 years. The map projection is distorted at high northern latitudes because the mesh pole has been shifted into the boreal land mass.
Fig. 8. Vertical sections through the Fig. 7 results. The left-hand axis is in units of model layer number. The top six layers are each approximately 25 m thick. The lower axis is model cell number from south to north, through the center of the deposited field. Antarctica is excluded. Top — 2 months; bottom — 4 years.
Fig. 9. A three year partial ecology simulation in POP. Surface phytoplankton distributions are shown for the 3rd July (mmol m$^{-3}$). Labeled values are grid cell numbers. The map projection is distorted at high northern latitudes because the mesh pole has been shifted into the boreal land mass.
Parallel Ocean Program (POP) computations are already underway at a preliminary level. We have taken a 2/3° resolution spin-up run which is normally used to bring the thermohaline circulation into relative equilibrium, and have added several new tracer compartments. The standard code is full physics but contains no biogeochemistry, and so carries only temperature and salinity as advected quantities. We have, thus, taken advantage of POP's ability to handle an arbitrary number of tracers. With the new tracers that have been added, we have been able to perform advection and upwelling tests analogous to those described above for the idealized Stommel code. The spin-up model contains the standard POP vertical structure—32 levels in depth coordinates. The layers are 25 m thick near the surface and become broader in the abyss.

In an early set of POP runs, a finger of inert material was injected daily into the Western Pacific as a tracer beyond temperature and salinity. The substance was permitted to move with the major current systems for 4 years (Fig. 7). It may be viewed as an arbitrary pollutant carried on the geostrophic westerly winds from Asia. The effect of the Kuroshio is apparent, and currents outside the subtropical gyre also play a role. Transport took place from the general area of the Indonesian Archipelago southward and eastward with the equatorial countercurrent. Vertical sections (Fig. 8) showed that the tracer eventually penetrated to several hundred meters depth at mid latitudes. In a second group of tests we have added partial ecology to POP. 150 m nitrate levels from the Levitus et al. (1993) compilation rise and are converted to biomass. Fig. 9 displays global phytoplankton distributions at the surface for the third July in a three year simulation. The major patterns for this run are a spring–summer bloom that is apparent at high northern latitudes, and equatorial upwelling/production interacting with tropical eddy structures.

POP currently advects the tracers we have inserted in a centered leapfrog scheme (third-order upwinding is a recently added option). The leapfrog is known to be both dispersive and diffusive (Anderson et al., 1984). Ringing can artificially move material ahead of and behind bulk transport. We have observed these and other effects in advection tests, both in the Stommel ocean (McNair et al., 1998) and in POP. The eco-tracers we plan to deal with in some cases possess short removal time constants and so will present the horizontal transport routine with sharp gradients. Schemes more sophisticated than leapfrog are being considered in anticipation of further biogeochemical runs (Hecht et al., 1995).

7. Computations

Our ecology and dissolved gas chemistry modeling effort will be computationally intensive in several senses: (1) The need for discrimination of mesoscale eddies is currently driving the development of high resolution ocean models. Grid sizes on the global mesh are fast approaching 1/10° (Smith et al., 1992; Bryan et al., 1998). Our time constants suggest that the turbulence and ecchemistry will interact in crucial way at such scales. (2) As in studies of atmospheric photochemistry (Liu et al., 1987; Crutzen, 1988; Elliott et al., 1995, 1996), many tracers are coupled within the system of ordinary differentials. Distributions are thus difficult to treat individually. It could be said that the system requires enhanced resolution in all of the physical, ecological and chemical dimensions.

Our POP colleagues have described the parallelization of physics and transport routines for the standard quantities temperature and salinity. Under the concepts of time splitting the arguments extend directly to our tracers (Yanenko, 1971; Elliott et al., 1993). We have argued here that vector and parallel lengths under the dominant massive computer architectures are most likely to be exceeded in the ecology and chemistry routines with geographic indices prioritized. With these optimizations in force, we now offer timing statistics for our routines on a variety of machines. The data should provide the reader with guidance on computational requirements as similar coding is implemented elsewhere.

The one-dimensional and Stommel models have been run primarily on SUN work stations. The machine we have used most often is a SUN Ultra with a 64-bit SPARC I® microprocessor; 64-bit Sbus running at 25 MHz. Several days of wallclock time were needed to complete a physical year in the idealized, 3D circulation with ecochemistry (roughly 20 interacting tracers). The Parallel Ocean Program originally ran on the Los Alamos TMC-Connection Machines. For example, many runs were performed on the CM-5, a massively parallel SIMD computer with 2048 64-bit floating-point processors and 8 Gbytes of core memory. The CM-5 had a 10 MHz clock. Our programs were never timed upon it. Currently POP is running on the SGI/Cray Origin2000. The Origin is a RISC-based machine, running the Cellular IRIX operating system. It currently has 128 processors, with MIPS RISC R10000 64-bit CPUs. We generally have access to only a fraction of the total capability. At 24 processors 15 min on the wallclock time are consumed to run a one month simulation in the 2/3° POP version. Ultimately 1024 or more processors will be available.

Latest versions of the ecodynamics and gas chemistry codes that we are developing can be obtained by
emailing requests to lead author Shaoping Chu (spchu@lanl.gov).

8. Summary

By constructing and applying a suite of marine ecology/chemistry/transport models, we are moving toward study of the coupled marine ecology and atmospheric chemistry systems. A bridge between ocean and atmosphere is formed by reactive dissolved gases, including DMS, OCS, the methyl halides and others (Andreae, 1986; Liss, 1986; Elliott et al., 1987,1989; Ratte et al., 1993; Andreae and Crutzen, 1997). The species are produced by organisms and dissolved organics, and are later consumed in the water column both biologically and chemically. They also transfer across the sea–air interface and influence gas phase photochemistry and climate. In the present paper, we introduce early versions of the ecochemistry models and we are applying to interpret their behavior.

The nitrogen ecodynamics that determine primary productivity in the open sea are described initially (Mann and Lazier, 1996), along with several prominent marine ecology models used to represent them (Fasham et al., 1993; Doney et al., 1995,1996). The connections with dissolved gas chemistry are outlined as well (Buat-Ménard, 1986; McNair et al., 1998). The ecodynamics and chemistry are related mathematically to one another and to ocean transport in a set of differential and finite difference equations (Sarmiento et al., 1993; Elliott et al., 1993). Prospects for exploiting parallel supercomputing capabilities and for automation of solutions are outlined. Placing geographic indices on inner loops allows full parallel lengths to be exploited (Levesque and Williamson, 1989; Elliott et al., 1993). The ecochemistry model we derive is already quite complex, treating about 20 tracers and several times that many reaction processes (Fasham et al., 1993; McNair et al., 1998). Automation will prove useful as the resolution of the ecological and photochemical systems is increased. In attempting to design stable and efficient marine gas chemistry coding we have drawn heavily on our experience with atmospheric photochemistry systems (Turco et al., 1979; Elliott et al., 1987,1989; Ratte et al., 1993,1995,1996). To large extent the computational approaches can be viewed as analogous. Structure of the ecodynamics/gas programs is exposed by listing major calls in the driver sequence, and the purposes of the related subroutines.

Results are shown from a series of increasingly sophisticated simulations. We begin with a simple one-dimensional, nitrogen based ecosystem model emulating Fasham et al. (1993). To it are appended production and loss processes for the volatile species. The latter are coupled among themselves as well as to the biology. The chlorination reactions of methyl iodide and methyl bromide, for example, create methyl chloride. The full ecology/gas chemistry routine has been inserted into an idealized, 3D basin circulation code (Stommel, 1948; Hecht et al., 1995). General features of observed oceanic nutrient upwelling and phytoplanktonic blooms are reproduced (Gurney et al., 1993). Biogeneration terms are adjusted for the gases to give realistic average concentrations. Ultimately, the ecochemistry will be inserted into the POP general circulation model (Semtner, 1986; Smith et al., 1992). Inert tracer advection and simplified ecology experiments have been performed in POP as preludes to transfer of the chemistry.

Early results are shown, and wallclock timing statistics are offered. The preliminary POP work indicates that computational demands will be manageable.

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