VIRTUAL

PLANKTON ECOLOGY

Using the primitive equations of marine physics, chemistry and biology to simulate the plankton ecosystem in the sea

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Chapter 3 Forcing

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3 Forcing

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Summary

A virtual plankton ecosystem is created by integrating a Lagrangian Ensemble model under prescribed conditions of forcing by external phenomena. There are five kinds of forcing: (1) ocean circulation, (2) initial conditions, (3) boundary conditions, (4) trophic closure, and (5) events. A VPE is sensitive to every kind of forcing, whether biological (e.g. trophic cascade or fisheries recruitment), chemical (e.g. nutrients or plankton multiplier) or physical (Woods-Onken effect or permanent oligotrophy). Uncertainty in forcing leads to systematic errors in the emergent properties of a VPE, reducing the value of predictions. So the designer needs to pay as much attention to forcing as to the model. Each kind of forcing is controlled by exogenous data which by definition - are unaffected by the state of the VPE. In practice, forcing is coded by selecting options displayed in the graphical user interface of the virtual ecology workbench. The VEW contains sample global data sets for this purpose. The VEW is an open system so the user can add alternative exogenous data sets.

3.1 Introduction

A virtual plankton ecosystem is created by integrating the model under prescribed forcing. Here we consider the forcing. It has five parts: (1) ocean circulation, (2) initial conditions, (3) boundary conditions, (4) trophic closure, and (5) events. Each of these involves an exogenous data set, which is unaffected by the state of the virtual plankton ecosystem. Sample exogenous data sets are included in the Virtual Plankton Workbench; but the VEW is an open system, so the user can easily substitute alternatives. Some of the exogenous data are regional (e.g. for the North Atlantic), but others are global, allowing the modeller to simulate the plankton ecosystem anywhere in the world ocean.

That is important when the virtual mesoscosm (which contains the VPE) drifts with the ocean circulation. A typical numerical experiment simulates change in the ecosystem over several decades. During that period the mesocosm's track can span an ocean basin. The track is computed by integrating an exogenous data set comprising a 4D velocity field derived from an ocean general circulation model.

The initial conditions define the state of the VPE at the start of that track. Values are required for every state variable of the model in every layer of the mesocosm. They are obtained from an exogenous data set derived from historical observations. They may be station data from oceanographic experiments like WOCE (the World Ocean Circulation Experiment) or they may be climatological compilations assembled from all available historic data (e.g. the NOAA Ocean Climatology).

The boundary conditions comprise vertical fluxes through the top of the virtual mesocosm, i.e. through the sea surface. Some of the fluxes are unaffected by the state of the VPE: these include the downward irradiance of sunlight (insolation), and the precipitation of water (rain, snow) or dust. Other fluxes depend of the sea surface temperature (in the top layer of the mesocosm); these include conduction of heat, evaporation and thermal radiation. The fluxes of gases through the sea surface depend on the saturated vapour pressure of the gas in solution (which is controlled by both temperature and the concentrations of dissolved chemicals). In addition to these endogenous properties of the VPE, the fluxes depend on the state of the atmosphere (cloud cover, air temperature and humidity, and partial pressure of gases). These

exogenous properties are derived from historical observations of meteorological observations collected for weather forecasting. In the past they were combined statistically (e.g. Bunker), but more recently they have been assimilated into a weather forecasting model (e.g. ERA40).

The fourth kind of forcing is trophic closure. Changing it affects the demography of all the plankton species in the VPE and biofeedback modifies the environment. Trophic closure is effected by top predators eating zooplankton that are modelled explicitly (by computer agents) in the VPE. The top predators are members of the model plankton community, but they have special properties. Their predation rate depends on two factors, one endogenous, the other exogenous. The endogenous factor is the top predator's phenotypic rule for ingestion, which is similar to those of the explicit zooplankton. The exogenous factor has two parts, biological and demographic. The biological part is the predator's size (biological condition). The demographic factor is the number of top predators in each mesh cell. Both the biological and demographic factors are prescribed as time series with values for every time step of the VPE's existence.

The final kind of forcing is concerned with prescribed events, which modify either exogenous or endogenous properties at prescribed times. One example of an exogenous event is the secular rise in atmospheric carbon dioxide concentration that has been observed during the last century and is predicted to occur during this century. An example of prescribed changes to (endogenous) state variables of the VPE is a pollution event in which chemicals are injected into the sea over a range of depths. Another example is the introduction of alien species of plankton contained in ballast water flushed from an oil tanker. Events may be specified as part of the forcing with a view to simulating a real or hypothetical happening. Or the motivation may be to learn more about the nature of the VPE by deliberately perturbing it.

The exogenous data sets used to force virtual plankton ecosystems typically have a spatial resolution of one degree of latitude and longitude $(1^{\circ}x1^{\circ})$, or a box of one hundred kilometre sides at mid-latitude). A one-dimensional VPE represents the average conditions in a box of those dimensions. For convenience we imagine a one-dimensional virtual ecosystem contained in a mesocosm that has a horizontal cross-section of one square metre, but as we noted in chapter 2 the (vertically-integrated) plankton demography has units of plankters per square metre. Looking to the future,

we shall have access to velocity fields with much finer spatial resolution, perhaps 1km x 1km at fronts. These will represent mesoscale turbulence. Using a larger mesocosm with a three-dimensional mesh for the environment and allowing the plankton agents to have 3D trajectories, it will be possible to simulate plankton patchiness within the mesocosm. However, the forcing will still have a resolution of $1^{\circ}x1^{\circ}$. The plankton ecosystem will still represent the mean conditions in that box, including the mean patchiness due to mesoscale turbulence.

The following sections of this chapter examine the five kinds of forcing. §3.2 considers the requirement. Forcing is designed to support three different tasks: forecasting, hindcasting and what-if? prediction. The most important of these is hindcasting, which underpins the other two. §3.3 introduces the exogenous data sets that support hindcasting; they are derived from historical observations. The Virtual Ecology Workbench (§3.4) contains a default set of exogenous data that allow the modeller to create a virtual ecosystem anywhere in the world ocean. The VEW is an open system that allows users to substitute alternative forcing data. There follow five sections reviewing issues involved in selecting and using exogenous data for hindcasting: §3.5 circulation, §3.6 initial conditions, §3.7 boundary conditions, §3.8 top predators, and §3.9 events. All the data sets have errors that induce uncertainty in VPE hindcasts; they are discussed in §3.10. The chapter ends with a conclusion (§3.11).

3.2 Requirements

All virtual plankton ecosystems are, in a sense, predictions. They show how the plankton community responds to its changing environment, which is controlled by a combination of forcing and internal processes including biofeedback. However, VPE prediction seldom addresses *forecasting* for reasons given below. The most fruitful kind of prediction is *hindcasting*, which provides the basis for *what if? prediction*. The three kinds of VPE prediction will be discussed below.

3.2.1 Forecasting

Forecasts are designed to reveal how a VPE will develop in the future: they require a weather forecast for surface flux forcing. To achieve an effective forecast, the VPE must start in a balanced state, i.e. it must be on attractor at the start of the forecast.

(Lynch 2006) reminds us that the failure to start with a balanced state is fatal, as it was for (Richardson 1922)'s pioneering numerical weather forecast. A numerical weather system can be brought to a balanced state in less than one simulated day using global observations collected at the starting time. That is the basis for modern weather forecasting.

However, it is not possible to balance a virtual plankton ecosystem so quickly. There are two reasons. The first is that it is not yet possible to collect a sufficiently detailed synoptic observation of the plankton ecosystem. The second is that, were such observations technically possible, they would describe the real ecosystem in the ocean, rather than the simpler model ecosystem with its severely truncated community. We shall see in chapter 11 that there is another way to achieve a balanced state in a virtual plankton ecosystem. This involves allowing the VPE time to adjust to an attractor, which is independent of the initial state of the ecosystem (other than nutrient concentrations). The problem is that adjustment takes several years, because it depends on demographic changes in successive growing seasons. And exogenous forcing must be sustained throughout the years of adjustment. The final state is in balance with that history of forcing, on the one hand, and the model plankton community, on the other. The history of forcing ends on the day when the forecast is due to start. This yields the best possible description of the VPE at the start of the forecast. Paradoxically, the initialization would deteriorate if one attempted to assimilate current synoptic observations. That is because they would describe the state of the real rather than the model ecosystem. Assimilating contemporary observations (e.g. ocean colour) would disturb the VPE, pulling it off the attractor that had be carefully established from forcing during the previous few years. If the goal is to forecast the plankton ecosystem for a few days ahead, initial balancing is best achieved by forcing the VPE with historical data extending back upstream for several years.

3.2.2 Hindcasting

Hindcasting lies at the heart of virtual plankton ecology. It uses historical observations to compute the forcing. There are two strategies: (1) assuming a stationary annual cycle in forcing, and (2) following the sequence of forcing in successive years. The first option has been the forcing of choice for numerical experiments designed to isolate internal fluctuations in the ecosystem, as in (Woods

2005; Woods, Perilli et al. 2005). It is useful when developing a new VPE. Note that while this forcing has a stationary annual cycle in each geographical box $(1^{\circ}x1^{\circ})$ the cycle varies with geographical location. So a drifting mesocosm samples a different annual cycle at each location along its track. Numerical experiments with this kind of forcing allow the modeller to discriminate between the impacts of geographical climate change and inter-annual variation in the weather.

The second option uses the six-hourly meteorological data generated by re-analysis of archived synoptic meteorological observations (ERA40 or NCEP). These data extend over forty years (longer in the future). They allow the modeller to create a VPE for any period in that range, knowing that the atmospheric forcing follows the actual conditions at the changing location of the drifting mesocosm. This opens the door to simulating inter-annual variation, with the ecosystem responding to past weather systems. Ideally, the other kinds of forcing should also have the synchronized long time series. The first step in that direction is to create a 4D velocity field with realistic inter-annual variation by using the ERA40/NCEPS meteorology to force the ocean general circulation model. However, initial conditions must remain annual means because high seas archive data do not support inter-annual re-analysis.

3.2.3 What-if prediction

Hindcasting provides the platform for *What-if? Prediction* (WIP). The strategy is first to establish a default VPE with the most realistic forcing available. In IPCC terminology this is "Business as Usual" forcing. Then the modeller creates modified VPEs each featuring an event that alters the forcing. The events may be continuous (such as a progressive rise in ApCO₂), or short-lived (such as a pollution incident). The aim is to discover how the virtual ecosystem responds to different events, each specified at a range of intensities.

The primary aim of such perturbation experiments is to improve understanding of a VPE. But when that has been achieved, they can be applied to operational oceanography. There are two kinds of forcing in this application of WIP. The first simulates the ecological problem, for example a harmful algal bloom. The second overlays various scenarios for remedial action. The results can be useful in training environment protection staff on the likely consequences of various courses of action, including doing nothing.

3.3 Exogenous data

It is important to keep separate the model and forcing in the specification for a virtual plankton ecosystem. That is done in the VEW. The distinguishing feature of forcing is its associated exogenous data. By definition, exogenous data are not influenced by the state of the ecosystem. In reality they may be. For example, inter-annual variation in the seasonal cycle of chlorophyll concentration modifies the spacing of isotherms in the seasonal thermocline, and therefore the isopycnic potential vorticity. This effect is strongest during the spring bloom, which typically subducts isotherms in the depth range 100 to 30 metres. The water in the permanent thermocline in ventilated from the lower layer of the seasonal thermocline. Its profile of potential vorticity influences the ocean circulation. So there is a connexion between inter-annual variation in the spring bloom and ocean circulation. This link can be quantified by numerical experiments with virtual plankton ecosystems. In practice the response of the ocean circulation to the plankton ecosystem is small on time scales of decades. This biofeedback can safely be ignored in most VPE investigations.

3.3.1 Sources of exogenous data

Every data set used for forcing is derived from archives of observations made in the past, mainly during the 20th century. Climate is changing faster than ever before, so hindcasting must be treated with caution when verifying a VPE against observations collected in the 21st century. There is a danger that our understanding of the plankton ecosystem based on diagnosis of VPEs will become misleading. Consider, for example, the substantial changes in distribution of calanoid copepods documented by the CPR¹ surveys in the 20th century (Beare, Gislason et al. 2002). It is therefore important to use the latest available data for forcing VPEs. The VEW is an open system that allows modellers to upgrade the exogenous data listed in table 3.1.

The data sets used for VPE forcing have been compiled at considerable effort by specialist institutions. The most complete global oceanographic data set was collected by the World Ocean Circulation Experiment (WOCE, 1985-95). These high quality hydrographic observations, which include nutrients, can be used directly to initialize

¹ Continuous plankton recorder, which is operated by SAHFOS (the Sir Alister Hardy Foundation for Ocean Surveying), operates CPR surveys to monitor the plankton ecosystem around the world.

VPEs at station locations. Data collected by the 21st century Global Ocean Observation System (GOOS) is used to initialize ocean circulation models that produce velocity fields useful for forcing VPEs. But GOOS data do not yet include nutrients, so they cannot be used to initialize VPEs. So it is necessary to rely on archive data accumulated over many decades.

The first stage is to compile the observations and allocate them to space-time bins. These are typically 1°x1° at intervals of 12 hours (meteorological observations), or one month (oceanographic observations). In some regions, the data are so sparse that the observations are all put into the same time bin, regardless when they were collected. Observations made during oceanographic cruises tend to be biased to the summer and Northern hemisphere. The temporal bias is particularly worrying for variables, like nutrient concentrations, that exhibit strong seasonality (summer oligotrophy); we shall discuss this problem in §3.12.

The binned data are then processed to produce a regular gridded data set for use in virtual plankton ecology. The first step is fill gaps in the binned data set by interpolation. Different data sets are then processed in different ways. The classical method is statistical: yielding a mean value in each bin. The VEW provides North Atlantic surface climatology derived from ship meteorological observations collected by (Bunker 1976) and reanalyzed by (Isemer and Hasse 1987). (Baumgartner and Reichel 1975) used the same technique to create the surface water flux climatology. More recently, similar methods are used to create maps of sea surface variables (temperature, wind waves, dynamic pressure) from satellite observations (REF).

The modern method of processing observations involves assimilating them into a dynamical model of the atmosphere or ocean, creating a dynamically-balanced simulation, then extracting the emergent properties needed to force the VPE. This method was pioneered by meteorologists, who produced two widely used *re-analysis* data sets: ERA40 and NCEPS. These benefit from international agreement to collect observations at fixed times each day, although the spatial distribution is uneven on land and sparse at sea. Systematic observations from satellites have largely overcome those inhomogeneities.

The 20th century archives of oceanographic observations do not benefit from internationally-coordinated synoptic sampling. The data assimilated into ocean

circulation models have usually been binned over decades. Nevertheless the FRAM² project showed that the physical environment of the "virtual" ocean does eventually settle to a balanced state – an attractor – with emergent properties suitable for use in forcing a virtual plankton ecosystem (Fram-Group 1991/9/April).

3.4 The Virtual Ecology Workbench

The forcing data sets contained in the VEW are summarized in Table 3.1. The VEW can display any of these data as maps. The mesocosm track can be overlaid on these maps. This facility is useful in planning a numerical experiment.

² Fine Resolution Antarctic Model. See the FRAM AtlasFram-Group, T. (1991/9/April). "An Eddy-Resolving Model of the Southern Ocean." <u>Eos, Transactions, American Geophysical Union</u> **72**(15): 174-175.

Table 3.1 Exogenous data sets in VEW4				
Source	Variable	Horizontal resolution	Vertical resolution	
World ocean climatology (NOAA)	Temperature, salinity Nutrients (N, P, Si) Plankton Mixed layer depth	1° x 1°	Standard depths	
OCCAM (NOCS)	Velocity vector (monthly mean)	0.25° x 0.25°	Standard depths	
ERA40 met data (ECMWF)	 (1) synoptic data every 6 hours (2) 40y synoptic mean at six hour resolution (3) 40y monthly mean 	1° x 1°	 (1) Cloud cover at standard level (2) Wind, temperature, humidity at standard height above sea level 	
<i>ERA40 fluxes</i> (ECMWF)	Sensible heat, latent heat, net IR, momentum, precipitation	1° x 1°	Sea surface	
<i>BRA</i> (IFM Kiel)	Sensible heat, latent heat, net IR			
<i>TP1 non-visual</i> (Functional group representing all non-visual predation on herbivores.)*	Seasonally-varying demography (TP/m ³) and biology (individual size in molC)	-	In each layer of the mesocosm mesh.	
TP2 visual (Squid)*	Seasonally-varying demography (TP/m ³) and biology (size of individual TP expressed in molC)	As available in fisheries surveys	In each layer of the mesocosm mesh.	

Notes for Table 3.1

NOAA	USA National Oceanographic & Atmospheric Administration		
ECMWF	European Centre for Medium-range Weather Forecasting		
Squid	References in (Sinerchia, Vallerga et al. 2008)		
Standard depths	(1) NOAA climatology xxx		
	(2) OCCAM circulation xxx		
Top predators*	The exogenous data used to specify top predators depend on the		
	species included in a particular model. The sample VPE included in		
	the DVD is based on the LERM model (Sinerchia, Vallerga et al.		
	2008). It has two top predators: (1) visual, with seasonally-varying		
	demography and biology, and (2) non-visual, with constant biology		
	and steady, homogenous demography.		

3.5 Ocean circulation

The track of a drifting virtual mesocosm is computed by integrating a fourdimensional velocity field derived from an ocean general circulation model (OGCM). The VEW contains a global velocity field with a spatial resolution of ¹/₄° with values at monthly intervals during one year. It was created with atmospheric forcing for 1996, but it is treated as a stationary annual cycle for as many years as is needed. The VEW is an open system, so there is scope for substituting new velocity fields as they become available.

3.6 Initial conditions

The initial conditions comprise values for every state variable in the model at every level in the mesocosm. They are a necessary part of the specification for a new VPE. The computer run cannot begin without them. However, most of the initial conditions are merely scaffolding to get the run going. After an initial period of adjustment, usually a few years, the model and forcing will get into balance, the VPE will then be on attractor. The properties of that attractor do not depend on the initial scaffolding. So the choice of initial values is not important. (Woods, Perilli et al. 2005) showed that the initial size of the plankton populations can be doubled or halved without affecting the demography of each population when it is on attractor. The same goes

for the initial physical conditions, for example the mixed layer depth. However the chemistry is different.

The initial concentrations of nutrients are not scaffolding. They define the resources available for biological production. (Woods, Perilli et al. 2005) plotted the change in the attractor with increasing initial nutrient concentration in the winter mixed layer. It is therefore important to find a reliable source of data for the nutrients at the starting time and location of the virtual mesocosm. One option is to initialize the VPE run at the location of a hydrographic station where the nutrient profile was measured, for example during WOCE. Another option is to base the initial nutrient profile on the NOAA climatology, interpolated to the starting location.

It is normal practice to initialize a VPE in winter when the plankton are quiescent, and each population has its annual minimum number. The annual maximum depth of the mixed layer is attained at the end of the winter cooling season. This is the time of year when nutrients sequestered in the seasonal thermocline have been re-entrained into the mixed layer. So initialization requires a value for the nutrient concentration in the mixed layer at the end of winter. It is very rare to find ship observations at that time of year. However nutrient measurements can now be made with sufficient accuracy by unmanned instruments mounted as payload on autonomous vehicles which can roam round the ocean in the winter mixed layer, and deep enough to avoid disturbance by wind waves. So winter nutrient data suitable for initializing VPEs will become available during the 21st century.

3.7 Boundary conditions

The boundary conditions comprise fluxes through the interface between atmosphere and ocean, at the top of the mesocosm. The fluxes are solar radiation, precipitation of water and dust.

3.7.1 Solar radiation³

Insolation is defined as the downward flux of solar radiation at the top of the mesocosm. The Virtual Ecology Workbench adopts the 25 waveband spectrum of (Woods, Barkmann et al. 1984). It ranges from the UV (xx wavebands) to the IR (xx wavebands) and includes 12 wavebands in the photosynthetically active range (PAR, 400-700nm); see table 3.1. The whole spectrum is used to compute the profile of downward irradiance. Solar heating is computed from the vertical divergence of this flux. The PAR spectrum is used in LE models to describe the action spectra for pigments used in photosynthesis and vision.

The VEW treats solar radiation as a beam, which suffers losses during its passage through the atmosphere and at the sea surface, where it is refracted. No account is taken of diffuse light entering the ocean. The direct beam of solar radiation approaches the sea surface at an angle to the vertical (solar elevation). The solar elevation changes with the geographical location of the virtual mesoscosm, the time of day and the day of the year. It is computed from astronomical formulae (Paltridge and Platt 1976), which are embedded in the VEW kernel. The computation is performed on the fly for each time step as the model is integrated to produce a virtual ecosystem.

Solar radiation is substantially modified as it passes through the atmosphere. The Workbench uses a rather simple treatment based on (Woods, Barkmann et al. 1984), see also (Woods 1980) and (Woods and Barkmann 1986). It computes solar radiation as a beam that approaches the sea surface at the solar elevation. The irradiance in each waveband takes account of losses in the atmosphere. The model does not include diffuse radiation from light that has been scattered in the atmosphere. The reduction of irradiance due to clouds is based on the three-level cloud-radiation model of (Paltridge and Platt 1976). The model also computes losses to the direct solar beam caused by dust and water vapour. The loss of direct beam irradiance due to reflection

³ General references: Dobson, F. W. and S. D. Smith (1988). "Bulk models of solar radiation at sea." <u>Quarterly Journal of the Royal Meteorological Society</u> **114**: 165-182., Paltridge, G. W. and C. M. R. Platt (1976). <u>Radiative processes in meteorology</u> and climatology. Amsterdam, Elsevier., Mobley (19xx),

at the sea surface is computed using a fixed value for the albedo (i.e. ignoring spectral change around dawn and dusk; see (Payne 1972)). The vertical irradiance below the sea surface is corrected for refraction between air and sea. The optical code in the VEW does not include a functional relationship between sea state and light scattering at the sea surface.

(Liu and Woods 2004) used a much more detailed treatment of solar irradiance to predict ocean colour from first principles. It included explicit treatment of scattering in the atmosphere and by waves on the sea surface. This scheme was used to compute the spectrum of upwelling solar radiation at the sea surface (i.e. ocean colour) for a virtual ecosystem at the Azores. It will be incorporated into a future version of the Virtual Ecology Workbench as an option for computing insolation (see Ch 6).

Some of the light entering the sea is scattered back out. The fraction is tiny: the sea is famously dark, especially in the open ocean. Most of the light we receive when we look down on the ocean comes from reflection at the surface; this is described by the albedo, which is about 6% at noon. The blue colour of the sea comes from reflection of diffuse skylight. But about 94% of the photons enter the sea; that is the insolation. They are scattered or absorbed by the seawater and by particles, especially the phytoplankton. A tiny fraction of the photons have their trajectories turned round by single or multiple scattering events, so that they pass back upwards through the water and exit through the top of the mesocosm. Most of this flux of upwelling photons turns round within the top ten metres of the water column; a tiny fraction reach a depth of thirty metres. (Liu and Woods 2004) modelled this process in a virtual plankton ecosystem. They used a Monte Carlo technique to simulate the trajectories of a billion photons in each of 25 wavebands. The spectrum of downwelling light changes with depth according to the concentration of pigments (mainly chlorophyll) in the phytoplankton. (Liu and Woods 1998) verified the computed spectrum of downwelling irradiance (the photons absorbed inside the sea at different depths) by comparison with observations during the BOFS⁴ spring bloom experiment (Savidge, Turner et al. 1992). They then computed the seasonal variation in the spectrum of upwelling light, which defines the ocean colour as monitored from space by the SeaWiFS satellite. That leads to our final point in this section on insolation. Ocean

⁴ Biogeochemical ocean flux study

colour is due to the re-emergence of a minute fraction of the light entering the sea. Neglecting that loss would produce a small error in the computed irradiance profile inside the sea, but the error is negligible for our simulation of the plankton ecosystem. For all practical purposes, the computation of forcing by solar radiation can ignore the response of the ecosystem. That simplification does not apply to the other fluxes through the sea surface, which we discuss in the next section.

3.7.2 Precipitation

(Baumgartner and Reichel 1975) provide a climatology of precipitation over the ocean derived from merchant ship observations. Satellite maps of, for example, Saharan dust plumes over the North Atlantic have been used to map the precipitation onto sea surface (REF).

3.7.3 Air-sea interaction

These fluxes differ from insolation and precipitation; they depend on the state of the ecosystem. They are computed from the states of both the atmosphere and the upper ocean. The Virtual Ecology Workbench uses conventional bulk formulae to compute the surface fluxes (see Box 3.1). They can be found in standard textbooks on atmospheric optics, air-sea interaction (e.g. (Kraus and Businger 1994), (Josey, Kent et al. 1998)) and in monographs dealing with the upper-ocean boundary layer, such as (Kraus 1977), (Soloviev and Lukas 2006).

Box 3.1 Bulk formulae used in the VEW to compute fluxes of heat, water and gases				
Momentum	[N/m ²]	$M = d_a \cdot C_m \cdot U$		
Power into turbulence	$[W/m^2]$	$P = M \cdot U$		
Sensible heat	[Cal/m ²]	$S = d_a \cdot C_h \cdot U \cdot (T_a - T_s)$		
Evaporation	$[mH_20/s]$	$E = d_s \cdot C_e \cdot U \cdot (Q_a - Q_s)$		
Latent heat	[Cal/m ²]	$L = L_{e} \cdot E$		
Net IR	[Cal/m ²]	$R = C_r (T_s^4 - T_a^4)$		
Gases	[Kg/m ² s]	$G = C_g \cdot d_s$.		

Notes

Ζ	[m]	The height above sea level. Upward fluxes are positive.
М	$[N/m^2]$	The momentum flux or wind stress
Р	$[W/m^2]$	Power into turbulence in the mixing layer
da	[Kg/m ³]	Density of the air at 10m above the sea (approximately $d_s/1000$)
ds	[Kg/m ³]	Density of seawater (circa 1 tonne/cubic metre)
C_m	[-]	Drag coefficient; variation with sea state is ignored in VPE
U	[m/s]	Wind speed at 10m above the sea
Ce	[-]	Coefficient for evaporation
Ta	[K]	Temperature of the air at 10m above the sea
T_{s}	[K]	Temperature in the top layer of the mesocosm mesh
Qa	$[N/m^2]$	Water vapour pressure in the air 10m above the sea
Q_s	$[N/m^2]$	Saturated vapour pressure of seawater at the sea surface
Le	$[J/m^3]$	Latent heat of evaporation of water
Pa	$[N/m^2]$	Partial pressure of gas in the air 10m above sea level
$\mathbf{P}_{\mathbf{s}}$	$[N/m^2]$	Partial pressure of gas in the top layer of the mesocosm mesh

The VEW contains two data sets for computing the air-sea fluxes:

- *ERA40* The re-analysis of historic weather observations by the European Centre for Medium-range Weather Forecasting (Uppala, Kållberg et al. 2006). Some users may prefer to substitute the American equivalent, NCEP (Kalnay, Kanamitsu et al. 1996). See (Rutledge, Saha et al. 2008) for a recent review of re-analysis activity. These pioneering re-analysis data sets have a time resolution of six hours and a spatial resolution of one degree of latitude and longitude. There are ambitious plans for re-analysis data sets with much higher resolution, with some versions extending back into the 19th century (Rutledge, Saha et al. 2008).
- *BRA* The re-analysis of (Bunker 1976)'s compilation of North Atlantic ship observations by the Kiel Institut für Meereskunde (Isemer and Hasse 1987).

3.7.3.1 ERA40

As we noted in §3.1 most of the numerical experiments performed in virtual plankton ecology are hindcasts. They simulate the ecosystem as it was during some period of years in the past (given the limitations of the model). The workbench includes a global weather data for the forty-year period 1959-1999. This data set, called ERA40, was created at the European Centre for Medium-range Weather Forecasts (ECMWF) by re-analysing historic observations with a modern data assimilation scheme of the kind used in 21st century weather prediction (Uppala, Kållberg et al. 2006). (Lynch 2006) provides a useful summary of the methods used in creating ERA40. In America NOAA/NASA have created a similar re-analysis data set, NCEP (Kalnay, Kanamitsu et al. 1996). The European and American two data sets are regularly extended to later closing dates. They now reach 2005. The Workbench is an open system. Users can easily upgrade ERA40 as extended versions become available, or they can substitute the NCEP re-analysis data set. Bunker re-analysis (Isemer and Hasse 1987) followed a different approach to re-analyse historic atmospheric data. They did not use the dynamical data assimilation in a numerical weather prediction model used to produce ERA40 and NCEP. Instead, they applied classical statistical analysis to re-analyse (Bunker 1976) compilation of North Atlantic meteorological observations collected by merchant ships during the period 19xx-19xx. The resulting Bunker Re-Analysis (BRA) data set has been used extensively in virtual ecology, e.g. (Woods 2005). It is embedded in the workbench, where it provides an alternative to ERA40 when the virtual mesoscosm is located in the North Atlantic. BRA provides a monthly-mean data set for surface fluxes with a spatial resolution of one degree of latitude and longitude. Its value will be discussed below (see §2.3.2.2 *Climate*).

3.7.3.2 Synoptic weather in the past

We have seen that ERA40 and NCEP have a temporal resolution of six hours. So they describe the synoptic weather in the past. The data set includes the cloud cover, which is used to compute how solar radiation changes as it passes through the atmosphere. The data set also includes the raw atmospheric variables at the bottom of the atmosphere: air temperature, humidity, wind speed and direction. These are used to compute the air-sea fluxes of momentum, sensible and latent heat, thermal (long-wave) radiation and evaporation.

The re-analysis data sets also include the synoptic sea temperature. The ERA40 data set includes air-sea fluxes computed from this sea surface temperature. The latter may vary slightly from the values computed using the emergent sea surface temperature of a virtual ecosystem. But, in practice the error is likely to be small, and the ERA40 fluxes are often used as boundary conditions for a virtual ecosystem.

3.7.3.3 Mean annual cycle

Many numerical experiments in virtual ecology require a stationary annual cycle of boundary conditions. The stationary annual cycle of atmospheric forcing is derived from averaging a re-analysis data set over all years to provide a single mean value of each surface flux and cloud cover at each time interval. The Workbench provides three versions of this climatology. Each has a spatial resolution of one degree of latitude and longitude. The first is the Bunker Re-Analysis (BRA), which has monthly mean values. The second and third are derived from ERA40. The second has the same monthly mean resolution as BRA. The third retains the full temporal resolution of ERA40, namely 40-year mean values of surface fluxes and cloud cover every six hours.

3.7.4 The endogenous component

Air-sea interaction depends on the state of the ocean as well as the atmosphere. Published climatologies compute the fluxes from synoptic observations of both systems. The VEW contains such surface flux climatologies from BRA and ERA40. However, the observed sea surface temperature and a VPE emergent surface temperature are not identical. The latter is sensitive to variation in seawater turbidity as the phytoplankton population waxes and wanes. The range of biogenic SST anomaly is a few Kelvin degrees. Ignoring this effect contributes significantly to the uncertainty in climate predictions (Woods 1984).⁵ It might be thought that it is best practice to compute surface fluxes from exogenous meteorology and endogenous sea surface temperature. If so the fluxes cannot be computed in advance: they must be computed on the fly during the computer run that generates the VPE. The VEW includes that option. However, it comes with a health warning. The ERA40 synoptic (6-hourly) meteorological data sometimes produce fluxes that are obviously erroneous (e.g. the wrong sign). Careful editing is needed before basing air-sea interaction on VPE emergent sea surface temperature.

3.7.5 Gases

(Liss and Slinn 2002) provide a recent account of the physics of air-sea gas exchange. (Woods and Barkmann 1993) used the bulk formula in Box 3.1 to compute the flow of carbon dioxide through the sea surface. The secular rise in the atmospheric partial pressure of carbon dioxide is documented by the time series of observations at Mauna Loa and elsewhere around the globe (Keeling, Piper et al. 2008).

3.8 Top predators

The top predators are planktivorous fish. They are modelled as functional groups with actual species or "mean" species. They feature in the model plankton community. They have phenotypic rules for ingestion, similar to those used for the explicit carnivorous zooplankton in the model. Time series of their size (used in computing ingestion rate) and demography (number of top predators in each layer of the mesocosm mesh) are exogenous data, which are computed beforehand (or on the fly during the integration) from exogenous top predator equations.

The model plankton community must include at least one top predator, which feeds selectively on one of the explicit zooplankton species. It may even feed only on one

⁵ This was the original motivation for the research programme on Virtual Plankton Ecology.

particular biological state of that prey species (for example one of its growth stages). In some model communities there are more than one top predator feeding on different zooplankton species. For example LERM (see ch.6) has two top predators: one feeds visually on the carnivorous zooplankton, the other feeds on the herbivores after catching them blindly.

The top predators are defined by the phenotypic rule and parameters for ingestion, and by the demographic equations and parameters for time series of their size and concentration. The model designer models each top predator on a species of planktivorous fish. The biology and demography come from the fisheries biology literature. For example, the visual top predators in LERM were modelled on squid, using data from (Boyle and Rodhouse 2005)'s monograph.

3.9 Events

An event may modify any of the VPE state variables at any time. The event is specified by entering details into the VEW graphical user interface. The specification depends on the planned numerical experiment. Often it will provide a perturbation to discover how the ecosystem responds. However there are some experiments in which the event is based on information from the scientific literature. Here are two examples. (Woods and Barkmann 1993) used the IPCC Business-as-usual scenario for the rise in ApCO₂ during the 21st century in their investigation of the plankton multiplier, which accelerates global warming. (Sinerchia 2007) treated squid spawning as an exogenous event in his investigation of fisheries recruitment: the date, depth and number of eggs laid were based on data in the fisheries literature.

3.10 VPE sensitivity to forcing

Virtual plankton ecosystems respond strongly to changes in forcing. The response affects all emergent properties of the environment and of the plankton. Those components are tightly bound together by the response of individual plankters to their ambient environment, and by plankton biofeedback to other plankton and to the environment. Here are some examples of VPE sensitivity to biological, chemical and physical forcing, imposed variously through trophic closure, initial conditions, boundary conditions and events.

There is an excellent literature on ecosystem response to change in top predators. This provokes a 'trophic cascade' which leads the ecosystem to adjust to a different attractor (Verity 1995). The phenomenon has been illustrated in a series of elegant controlled experiments in small Canadian lakes (Carpenter and Kitchell 1993). Similar changes can be demonstrated by biological events, for example spawning by fish that are exogenous to the VPE. The eggs are treated as an endogenous component of the plankton ecosystem. LE computer agents are used to follow their biology and demography. (Sinerchia 2007) performed numerical experiments to reveal the sensitivity of the attractor to the date of spawning and the number of eggs laid.

The VPE is equally sensitive to chemical forcing. (Woods, Perilli et al. 2005) plotted the change in attractor when the initial nutrient concentration was increased. (Arrese 2002) performed numerical experiments with chemical events (pollution injected into the seasonal thermocline). He showed that the timing of the autumn bloom is sensitive to the upward bio-transport of nutrients during summer oligotrophy. The transport is performed by diurnally-migrating herbivores that feed on phytoplankton in the deep chlorophyll maximum and are themselves eaten by carnivores in the mixed layer. A third example of VPE response to chemical forcing is the plankton multiplier (Woods and Barkmann 1993), in which the attractor changes in response to increasing inflow of carbon dioxide from the atmosphere. These three examples illustrate the ecological response to chemical forcing that acts through the initial conditions, an internal event, and boundary conditions (air-sea interaction) respectively.

Changes in physical forcing expressed through the initial conditions have no influence on the VPE after it has adjusted to the attractor. However the attractor is sensitive to changes in the physical boundary conditions: namely insolation, precipitation and airsea interaction. The direct impact is on the physical environment. Large changes occur immediately in the depth of the turbocline. This is seen most vividly in the diurnal cycle of insolation, which generates the laminar-flow regime in the diurnal thermocline with significant consequences for the phytoplankton (Woods and Onken 1982). It is also responsible for inter-annual variation in the onset of the spring bloom (Woods and Barkmann 1993). These are but two aspects of the complex response of the ecosystem to changes in the physical environment provoked by the diurnal and seasonal cycles of physical forcing; they are documented in (Woods 2005). That paper also shows how the transition from seasonal to permanent oligotrophy is provoked by geographical variation in physical forcing.

3.11 Errors

The exogenous data sets used to compute forcing are not perfect. Systematic errors in emergent properties of a virtual plankton ecosystem can be attributed in part to the inevitable measurement errors in the forcing data. Here we briefly consider the nature of those errors. Perhaps the word error is misleading: what we are really concerned with is how well the data represent nature; a better word would be uncertainty. The aim here is not to provide hard numbers for the uncertainty in forcing data; they will change in the future as new sources become available. Rather it is to raise awareness of the issues involved and to indicate how the errors might be assessed.

3.11.1 Ocean circulation

The ocean circulation data are used to compute the track of a drifting mesocosm. They are emergent properties from a simulation by general circulation model. The data set in the VEW was derived from an eddy-permitting (1/8° resolution) run of OCCAM. It comprises synoptic values at monthly intervals during one year of a multi-year simulation. All OGCMs have their strengths and weaknesses; but that is not our main concern here. Lagrangian integration of the velocity field yields a plausible track for the drifting mesocosm. The tracks presented in later chapters broadly meet expectations: the mesocosm circulates around the gyres, advancing faster in the western boundary current; and the presence of meanders and eddies sampled in the data set produce credible short-range displacements. So far so good; but the velocity field are shortcomings. First the velocity field, including the transient eddies, has a stationary annual cycle. Sometimes the mesocosm can become unrealistically trapped in an eddy for years before escaping to continue its migration around the gyre. So the modeller has to treat the tracks with caution.

3.11.2 Initial conditions

The computer run that creates a VPE is usually initialized in winter when the plankton are least active. So we need initialization data in winter when the mixed layer is deep. We noted earlier that while the model integration must be initialized with values for every state variable, only the nutrients affect the VPE when it has attained a balanced state; when it is on attractor. Unfortunately the oceanographic archives contain very few mid-ocean winter profiles of nutrient concentration. Seasonal oligotrophy makes summer profiles useless for initialization. The solution adopted for virtual plankton ecology has been to assume that nutrient concentration at the end of winter can be estimated by fitting a curve to summer observations in the permanent thermocline and extrapolating to the annual maximum depth of the mixed layer. This has obvious risks. Furthermore, the water near the top of the permanent thermocline was ventilated from the seasonal thermocline from a location upstream where the mixed layer last reached that depth. That location migrates meridionally with the severity of the winter. In harsh winters ventilation occurs nearer the equator where the nutrient concentration tends to be lower. Ideally one would make a correction for the year in which the data were collected, but that has not yet been attempted. To conclude, the nutrient profile in winter (used to initialize a VPE) is subject to substantial uncertainty.

3.11.3 Boundary conditions

The boundary conditions – fluxes through the sea surface - are all calculated from meteorological data. In some cases, for example (Bunker 1976), the data set was compiled statistically from observations. In other cases, the data were assimilated into weather forecasting model (e.g. ERA40 and NCEP).

Insolation. The computation of insolation is sensitive to the estimate of cloud cover. The BRA data contain subjective estimates of cloud cover by ships' meteorological observers. The ERA40 data are emergent properties of the meteorological model used to re-analyse past observations. Additional uncertainty arises from simplifications in the algorithm used to compute the influence of clouds (Liu 2003). These considerations suggest that there may be significant uncertainty in the computation of insolation. Nevertheless (Liu and Woods 1998) found good agreement between the computed profile of downward irradiance in the upper ocean, and BOFS observations.

Precipitation. The estimates of precipitation are, if anything, even more susceptible to error. On land the radar measurements of precipitation can be calibrated against rain gauges, but that is impossible at sea. However, the salinity anomaly in the seasonal boundary layer can be used as a kind of seasonal rain gauge (after allowing for evaporation). Using this technique, (Bauer, Leach et al. 1991) found remarkable

agreement with climatological maps of surface net water flux in the North Atlantic (Baumgartner and Reichel 1975), especially the transition between net annual influx and efflux of water.

Momentum (Chelton, Schlax et al. 2004) discuss the errors in satellite maps of wind stress and derived products like wind-stress curl. This source has largely replaced qualitative estimates from observations of sea state, although they are embedded in classical data sets such as BRA (Isemer and Hasse 1987) which are still used in virtual plankton ecology. The satellite data are generally considered more reliable than third source, meteorological re-analysis such as ERA40 and NCEP. There is a substantial literature on the impact of errors in wind-stress data on simulations of mixed layer depth and ocean circulation, for example (Chen, Busalacchi et al. 1994).

Evaporation and heat flux. Errors in wind-stress also contribute to the uncertainty in estimates of evaporation and heat flux. They also depend on values for air temperature and humidity, which are now best obtained from satellite (e.g. ATSR) or meteorological re-analysis ERA40.

Carbon dioxide. Errors in monitoring of atmospheric carbon dioxide are negligible for the purpose of hindcasting the sea-surface flux of carbon dioxide. But there is substantial uncertainty in the predictions of $ApCO_2$ published by the IPCC on the basis of socio-economic models. VPE research on the impact of the plankton ecosystem on climate tends to use the IPCC "Business-as-usual" scenario for the 21st century.

Trophic closure. When trophic closure is based on particular species of planktivorous fish like squid, the annual cycle of size and numbers comes from fisheries data, for which there are estimates of errors in the scientific literature (REFS). But there is little scope error estimation when the top predator is an idealized species designed to represent all the species in a particular functional group. In that case the modeller has little guidance on the range of uncertainty. This situation is worrying given the sensitivity of the trophic cascade to the specification of top predator.

Events. Numerical experiments involving events are normally performed in the spirit of *What-if? Prediction*, so the modeller has control over the range of values used in this kind of forcing.

3.12 Conclusion

This chapter has reviewed current practice in specifying the forcing of VPEs by exogenous phenomena. The forcing includes: (1) ocean circulation, (2) initial conditions, (3) boundary conditions, (4) trophic closure, and (5) events. The spatial resolution of the exogenous data is typically 1°x1°. That determines the spatial resolution of the virtual ecosystem. The requirement for forcing data depends on the motivation: forecasting, hindcasting or what if? prediction. Most investigations are concerned with hindcasting, in which the forcing is based on historical data. We reviewed the nature of those data and showed how they are used. The Virtual Ecology Workbench includes global exogenous data sets that it uses to generate forcing for one-dimensional VPEs anywhere in the world ocean. The VEW is an open system so users can substitute alternative data. Virtual plankton ecosystems are sensitive to changes in the biological, chemical and physical forcing. The chapter closed with a discussion of the errors in the exogenous data sets used to force VPEs. These errors produce uncertainty in the VPE emergent properties.

3.13 References

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