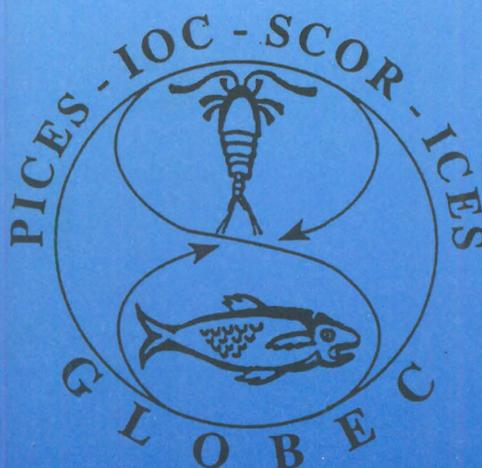


Coupled physical, chemical and biological models

by

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GLOBAL OCEAN ECOSYSTEM DYNAMICS

Belgian Globec Contribution Report n°6

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Abstract

The concepts underlying the construction of an interdisciplinary model are discussed. Two main aspects are emphasized : (i) state variables are defined by their nature (velocity, biomass ...) **and** their spectral window (i.e. their range of time and length scales), (ii) ecological variables generally represent aggregates (lumping together several elements belonging to some broad category, e.g. « phytoplankton »). One examines how these affect the interactions between physical and biochemical/ecological processes, the interactions between the latter and the mathematical formulation of the evolution equations which describe the variables' space-time dynamics. Two illustrative examples are given to show the type of information the present generation of coupled hydrodynamic/ecosystem models can provide.

Introduction

Ideally, a model should have four dimensions (time and three dimensions in space). A reduction of the dimensions can be achieved, however, by restricting attention to time and space averages, considering for instance (quasi) steady state models of low frequency residuals, depth-averaged models of shallow continental seas, cross-section averaged models of estuaries, time- and depth dependent models of surface and bottom boundary layers and of simple phytoplankton ecosystems, and finally box-models for completely space-averaged ecological, economic or management variables. Ideally, also, a completely realistic model should have an infinite number of state variables. Computing facilities, of course, impose limitations on the number of state variables but, independently of such restrictions, there are reliability and clarity constraints on the number of state variables. A model with many state variables incorporates as many different processes and interactions and involves a correspondingly large number of parameters and boundary conditions which cannot be evaluated from existing data bases without an inevitable margin of error. The results of such a model, on the other hand, - because of its increased sophistication and fallibility - can become impossible to interpret in terms of scientific diagnosis or management recommendations. **The essence of modelling is the selection of a limited number of representative state variables.** There must be sufficiently few of them for their evolution equations to be amenable to analysis but enough of them to describe adequately the system's behaviour.

The state space can be divided in several sectors corresponding to hydrodynamical, chemical, biological, economic ... models with the necessary input-output links between them. Of these, the hydrodynamic models are by far the most advanced. (In a sense, this is rather fortunate because the understanding of hydrodynamic processes is prerequisite to any form of chemical, biological or economic modellings and, indeed, constitute, in the present state of development of marine models, the most reliable contribution to the explanation and anticipation of ecological processes and to the management of marine resources). While *chemical, biological and economic models* are still frequently limited to *interaction box-models* describing, by means of *differential equations*, concentrations, biomasses ... in a hypothetical homogenous environment or averaged over large regions of space, *hydrodynamic models* have evolved to *transport-dispersion field-models*

describing, by means of *partial differential equations*, the spatial distributions and time evolution of field variables determined at all grid points.

Limiting the scope of the model to a particular sector of the state space reduces its dimensions. This can be achieved also by restricting attention to *aggregate averages* ; considering, for instance, zooplankton biomass (with no distinction between herbivores, carnivores and omnivores and, *a fortiori*, between species), total organic matter (lumping together dissolved and particulate organic matter), mercury concentration in fish (with no specification of its distribution), etc

One salient feature of the evolution equations which describe the transport, diffusion and alteration of marine environmental state variables is that they are fundamentally non-linear. This implies not only interactions between different state variables, but also exchanges between processes of different scales of space and time, associated with energy transfers actuating all the components of the spectrum. While non-linear interactions tend to spread processes over all scales, internal or external forcings acting on the system tend on the contrary to intensify particular components in ranges of scales corresponding to their own. The spectrum of a state variable is thus naturally made of a succession of peaks and valleys.

No model can represent the whole spectrum of events from molecular processes to climatic bifurcations. An essential characteristic of a model is thus its *spectral window*, i.e. the range of length scales and time scales which the model can represent. Quite evidently the spectral window of a model must always be defined so that it corresponds to the intense events associated with a peak. Smaller scale phenomena are not *resolved*. Their rapid variations take part in the *background of fluctuations* contributing to the diffusion or « smoothing » of the system's properties. Larger scale phenomena are not seen through the spectral window but are subjacent in the initial and boundary conditions.

This chapter is organized as follows :

- (i) In section 1, one examines the interactions between physical and biogeochemical/ecological processes and their mathematical formulation, taking into account the concept of spectral window.
- (ii) In section 2, one discusses the problem of selecting the appropriate set of state variables and formulating the interactions between them to provide an adequate

description of the biogeochemical and ecological complexity of the system and of its dynamics.

- (iii) In section 3, two examples of coupled 3D time-dependent models are presented and illustrated with applications. The objective here is not to single out one model rather than another, compare models or initiate a discussion on model validation, it is solely to display typical results of coupled models, to show the type of information these models can provide on the ecosystem space-time dynamics (even with a rather simple description of the ecosystem itself) and let the readers judge by themselves whether the product is worth the effort (or whether they would rather affect additional resources to the development of more sophisticated ecosystem box-models).

1. Natural variability, operant state variables and evolution equations

The natural variability of the marine system has long been recognized. Physical processes, forced by external (atmospheric ...) stresses and modulated by eigenmodes of responses to these stresses, which both have different length- and time-scales, display as a result of non-linear interactions a continuous spectrum of motions of all scales with peaks, -associated with external or internal forcings -, and valleys. Ecological and biogeochemical processes have, similarly, a scale-dependent hierarchical organization and many recent investigations have emphasized the possible *resonant* interactions of physical and biogeochemical processes of similar *time-scales* resulting in an adjustment of biogeochemical and ecological *length-scales* to the length-scales of the resonant physical processes, as a result of the permanent strain exerted by them on the system (e.g. Denman and Gargett 1983, Denman and Powell 1984, Steele 1985, Globec 1988, Denman et al 1989, Nihoul and Djenidi 1991, Nihoul 1993, Horne et al 1994, Denman 1994)*

As pointed out in the introduction, a model cannot address the whole spectrum of physical, chemical and biological processes and must focus attention on a specific spectral window. In this perception of the problem, state variables cannot be simply

* The *resonant* interaction of physical and ecological processes of *similar time-scales* determines the hydrodynamics processes which may significantly interact with the ecosystem. These processes maintain a permanent strain on the ecosystem which tends to impose to it the *length-scales* of the synchronous physical mechanisms. This is often referred to as the « *ecohydrodynamic adjustment* ».

defined in relation with their *nature* (fluid velocity, biomass ...). They must be further specified with respect to their time and length scales. The *operant* state variables of a marine environment model (denoted in the following by the generic letter y) are thus *mean values* representative of a specific spectral window (and may indeed be defined as time averages over a chosen time period T - corresponding to a spectral valley -, sufficiently large to filter smaller scale fluctuations and sufficiently small to let the phenomenon under investigation pass, unaffected, through the averaging procedure) (e.g. Nihoul 1993). The choice of a spectral window, i.e. the choice of T , is one defining feature of a model and, obviously, all the state variables of the model must correspond to the same spectral window, i.e. are similar averages over the same time T .

Considering interactions between physical and biogeochemical and ecological processes, one is thus led to make a distinction between the *flow* of y defined as the *transport* of y by the mean velocity \mathbf{v} (as defined above) and the *flux* of y summing up the overall contribution of the multiple and diversified displacements at scales not resolved by the model and viewed, on that account, as disordered fluctuations, generally associated with the *diffusion* of y . The equations describing the evolution in space and time of the state variables are then all particular expressions of a unique basic equation. This equation sets forth that the variation in time of any state variable (momentum, biomass, energy, ...), at any given point, is the result of (i) local production or destruction, (ii) divergence or convergence of the flow and flux vectors, i.e.

$$\frac{\partial y}{\partial t} = \mathbf{Q}^y - \nabla \cdot (\boldsymbol{\varphi}_0^y + \boldsymbol{\varphi}_u^y) \quad (1)$$

where \mathbf{Q}^y is the rate of production (destruction), $\boldsymbol{\varphi}_0^y$ is the flow, $\boldsymbol{\varphi}_u^y$ is the flux and ∇ is the vector-operator

$$\nabla = \mathbf{e}_1 \frac{\partial}{\partial \mathbf{x}_1} + \mathbf{e}_2 \frac{\partial}{\partial \mathbf{x}_2} + \mathbf{e}_3 \frac{\partial}{\partial \mathbf{x}_3} = \hat{\nabla} + \mathbf{e}_3 \frac{\partial}{\partial \mathbf{x}_3} \quad (2)$$

$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ denoting respectively the unit vectors along the axes of coordinates (\mathbf{e}_3 pointing vertically upwards), $\hat{\nabla}$ being the horizontal part of ∇ .

The flow of y is easily expressed in terms of the velocity \mathbf{v} of the ambient fluid as

$$\boldsymbol{\varphi}_0^y = y\mathbf{v} \quad (3)$$

The formulation of the flux is more subtle.

If the averaging time T is small (~ 1 sec), the sub-window scale processes are dominated by molecular diffusion and viscous dissipation of energy. The randomness of molecular agitation (which produces the diffusion) and the transfer of kinetic energy to a dissipation sink at small scales are two essential characteristics of the molecular diffusion range and it is well-known that molecular fluxes may be parameterized by the Fourier-Fick law, viz

$$\varphi_u^y = -\lambda^y \nabla y \quad (4)$$

If one considers averages over longer times T , one extends the sub-window range of scales to larger scales, including, as T increases, turbulence (possibly affected by vertical stratification), tides and storm surges, mesoscale eddies It is tempting to try to generalize eq. (4) to the corresponding fluxes. Whether this is acceptable or not will depend on the more or less random character of the sub-window scale processes and their ability to transfer kinetic energy to smaller scales where it is dissipated. Going from the smallest scales to the largest scales, marine geohydrodynamic processes tend to be more and more organized under the effects of external and internal forcings. The potential energy associated with these forcings plays a more and more important role as one goes to larger scales and transformations of one form of energy into the other provide more ways of energy transfers than the simple cascade of kinetic energy to smaller scales and ultimately the dissipation sink (e.g. Nihoul 1993).

Length scales increase with time scales but horizontal and vertical scales -which are the same order of magnitude in the small scales -, are more and more differentiated by the forcing mechanisms and the geometry of the ocean basins, and horizontal length scales become progressively, - as scales increase -, several orders of magnitude larger than vertical length scales (e.g. Monin et al 1977, Monin and Ozmidov 1985, Nihoul 1975, 1980, 1993).

Thus, (e.g. Nihoul 1993),

- i) smallscale turbulence (time scales form seconds to minutes) tends to be statistically homogeneous and isotropic and it is characterized by vertical and horizontal length scales of the same order of magnitude ;
- ii) in the vertical stratification dominated range (time scale between minutes and hours, denoted in brief as the « *mesialscale* » range in the following), vertical

scales are reduced by the stratification and, in shallow areas, limited by the depth ; the vertical and horizontal length scales of these components differ by one or two orders of magnitude, in general ;

- iii) in the mesoscale/synoptic range, the ratio of the horizontal and vertical scales is of the order nf^{-1} , where n is the Brunt -Väisälä frequency and f the Coriolis frequency ;
- iv) in large scale general circulation, the vertical length scale is limited by the depth while the horizontal length-scale reaches the dimensions of ocean basins.

In the scope of the Boussinesq approximation, the continuity equation reduces to

$$\hat{\nabla} \cdot \mathbf{u} + \frac{\partial v_3}{\partial x_3} = 0 \quad (5)$$

where $\mathbf{u} = v_1 \mathbf{e}_1 + v_2 \mathbf{e}_2$ is the horizontal velocity vector.

Eq. (5) is linear and must be satisfied by components of motion of all scales. Thus if ℓ_v and ℓ_h denote, respectively, characteristic vertical and horizontal scales and v_v and v_h corresponding velocity scales, one must have

$$v_v \leq v_h \frac{\ell_v}{\ell_h}$$

From small to large scales, v_h tends to increase but this is largely compensated by the decrease of the ratio ℓ_v/ℓ_h .

The choice of the averaging time T , defining the operant state variable y , determines the spectral window of the model and specifies which processes are treated as sub-grid scales and contributes to the fluxes.

- i) If T is such that the sub-grid scale processes include essentially smallscale turbulence and molecular effects, one may expect fluctuations' length and velocity scales of the same order of magnitude and comparable (essentially 3D turbulent) fluxes in the horizontal and in the vertical.

In the absence of significant ordering forces, the fluctuations are suitably random and the main energy transfer is to smaller scales and dissipation, as required for the diffusion model of fluxes (eq. 4) to be applicable.

Turbulent diffusivity coefficients can be expressed in terms of the kinetic energy of the turbulence k and its dissipation rate ε (or the related « mixing length » ℓ_0)

(e.g. Lumley 1978). Partial differential equations (in the general form of eq. 1) or algebraic relationships between k , ε and ℓ_0 can be derived from general principles and turbulence theory and there is a fairly general consensus now on the parametric forms and equations to be used in the present generation of 3D models with turbulent closure (e.g. Nihoul 1984, Blumberg and Mellor 1985, Rodi 1985, Nihoul and Djenidi 1987).

- ii) If T is such that the sub-grid scale processes comprise mesialscale, smallscale and molecular scale effects, horizontal and vertical fluxes include molecular, turbulent and mesialscale contributions (all averaged over T). From the discussion above, one expects horizontal fluxes to be dominated by irregular and versatile motions in the mesialscale range (large horizontal velocity fluctuations) and vertical fluxes to be essentially (T -averaged) turbulent fluxes. These fluxes will be affected by the restoring buoyancy forces but limited ordering and inhibition of turbulence by these forces are not, generally, sufficient to impede the globally diffusive and energy dissipating character of the fluctuations and fluxes can be parameterized on the model of molecular diffusion, allowing for different diffusivity coefficients in the horizontal (where the diffusion is dominated by mesialscale « fluctuations ») and in the vertical (where the diffusion is basically turbulent).
- iii) Moving the spectral window to still larger scales, one enlarges the sub-grid range to larger scale components. These will, by the same argument as above, contribute essentially to the horizontal fluxes and very little to the vertical fluxes which remain dominantly turbulent. Hence parametric form such as eq. (4) will presumably be still acceptable to represent vertical fluxes and vertical diffusion.

The application to horizontal fluxes is debatable. The processes which are associated with these fluxes are, - one may argue -, suitably chaotic, thanks to the multiplicity of energy sources, the variability of the forcings, repeated non-linear interactions and coastal reflections and may be described as « *fluctuations* » when viewed through larger-scale spectral windows. They are nevertheless impressed with the spatial structures and energy partitions of the forcings which always convey some form of organization to the system's hydrodynamics and allow energy transfers incompatible with the type of diffusion/dissipation model that eq. (4) transcribes.

Eq. (4) has been successfully applied to the model of the general circulation (and associated synoptic structures) of marine regions where tides were negligible and where the larger scale processes in the sub-grid range were essentially episodic and patchy flow events produced by wind forcings with lower-mesoscale variability (e.g. Nihoul et al 1989, 1993, 1994). In other cases (when the sub-grid range includes tides or synoptic eddies), equations like eq. (4) have been used (with eventually different diffusivity coefficients in the two horizontal directions), for lack of anything better, in preliminary investigations. There is no doubt however that a different approach is really needed when modelling macroscale processes with sub-grid scale fluctuations in the synoptic/mesoscale range. This approach requires the resolution of « *nested* » smaller scale models, resolving dominant sub-grid scale processes and (i) run in typical situations to provide a general guidance for the parameterization of the fluxes or (ii) interactively connected, through initial, boundary and assimilated data, with the larger scale simulation (e.g. Nihoul et al 1989, Delhez and Martin 1992, 1994, Globec 1993).

2. Natural complexity. Modelling biogeochemical and ecological interactions

One of the first steps in constructing an interdisciplinary model is the definition of a limited number of representative state variables. As pointed out in the introduction, there must be sufficiently few of them for their evolution equations to be amenable to analysis but enough of them to describe adequately the system's behaviour. This preliminary choice needs not be definitive and may be revised if one finds it necessary when validating the model, comparing hindcasting results with data or revising the model's objectives. Such revision, however, cannot increase the number of state variables beyond some « reliability » limit. A model with many state variables incorporates as many different processes and interactions and involves a correspondingly large number of parameters and boundary conditions which cannot be evaluated from existing data bases without an inevitable margin of error. The results of such a model, on the other hand, -because of its increased sophistication and fallibility -, can become impossible to interpret in terms of scientific diagnosis or management recommendations.

Classically, one begins by writing a *conceptual model* including as many variables and processes as one can think of. This model is usually presented in the form of a process flow diagram as the one shown in fig. 1. Boxes identify state variables, arrows

indicate interactions between them. One tries then to get a first assessment of the importance of the boxes and arrows by evaluating associated mean stocks and fluxes. Further examination of the data base provides orders of magnitude and, in particular, estimates of the rates of interactions which are essential to identify window scale and sub-window scale processes and appraise the sensitivity of the system to qualitative and quantitative modifications of the model's structure.

After this preliminary inspection and subsequent clearing of the model's flow chart, one must address the mathematical formulation of the interaction processes, the Q^y 's in eq. (1). No matter how frustrating it can be, if one doesn't have enough information to express the Q^y 's in mathematical form or to give reliable values to the parameters implanted in these mathematical formulations, or if suitable initial and boundary conditions are not available, corresponding pathways must be abandoned in the system's flow-chart and some appropriate closure must be devised to clog the model. This may require leaving out state variables and interaction processes or *aggregating* variables and processes. The aggregation procedure, mentioned in the introduction, consists in lumping together state variables belonging to some broader category and reformulating accordingly the interaction processes. In fig. (1), for instance, aggregates considered by Maloney and Field (1991) are underlined, boxes noted n_1 , n_2 , φ , β , z , d indicate furthermore aggregated variables as used in the modelling of the Northern Bering Sea by Walsh and Dieterle (Walsh 1988) and Nihoul et al (1994).

Decreasing the number of state variables by closing or lumping together path' ways, one obtains a smaller-size, hopefully tractable, model governed by evolution equations similar to eq. (1) but where the interaction rates Q^y 's must be formulated, mathematically, taking into account the surgery that has been performed on the model.

In general, Q^y may include :

- i) contributions of « *volume* » sources and interactions operating within the system and expressed as algebraic functions of time, space and state variables defined everywhere (e.g. the rate of decay of a radioactive substance, proportional to its concentration, the grazing rate of phytoplankton by zooplankton, a function of the two biomasses ...);
- ii) contributions of « *surface* » sources and interactions operating at the system's boundaries and expressed as algebraic functions of time, space and state variables

multiplied by a Dirac delta function concentrating their effect on the boundary surfaces (e.g. selective absorption of chemicals in surface films or even of radiation in the upper few meters of the sea can be represented as boundary sinks, inasmuch as bottom deposition of sediments, etc...);

- iii) in- and outfluxes contributing to the production rates, in differential form, through their divergences (e.g. sedimentation of heavy particles or ascension of lighter fluids are special cases of « *migrations* » corresponding to a production rate $-\nabla \cdot \phi_m^y$ where $\phi_m^y = \sigma y$ is the migration flux and σ the « migration velocity » ...).

The interaction rates must be determined from basic principles of Mechanics, Thermodynamics, Biogeochemistry, Ecology,

Transposing basic biochemical laws, calibrated in carefully designed and controlled laboratory experiments, to the complexity of the marine system is not, unfortunately, as straightforward as one would wish.

Models describe the evolution in time and space of *operant* state variables defined by their nature and their scales. The production/interaction rates to be substituted in the model's equation must be coherent with the state variable's definition.

- i) Models cannot describe every single organism, species, chemical compound ... simultaneously. To reduce the scope, one restricts attention to *aggregates*, lumping together for instance dissolved organic matter, phytoplankton, herbivores, nutrients ..., and *translocations* between them, - i.e. mass transferences in state space. The laws which are appropriate to describe translocations between aggregates must be inferred from chemical kinetics and marine biology, of which they are filiated products, but they are rarely straightforward transcriptions of them and their formulation is often not possible without a certain amount of empiricism.
- ii) Each model is characterized by its spectral window, i.e. the range of time and length scales it can resolve. The time scales of *natural* biogeochemical processes are not necessarily the same as the time scales of laboratory processes. One must thus be extremely careful in extrapolating laws and data from laboratory conditions to field conditions and models.
- iii) Laboratory experiments are often conducted in conditions (of concentrations, isolation ...) carefully chosen to magnify one particular process and observe it, in

the most intelligible way, in a reasonable time. These conditions may be very far from real field conditions and simple well-established theoretical laws explaining perfectly the laboratory observations may be totally inadequate in the sea.

For instance, unless one studies the dumping of high concentration material of well-defined composition in a marine sector where existing dissolved and particulate chemical's concentrations are known, and where simple laws of chemical kinetics may be expected to apply during a first post-dumping phase of -often violent and rapid - reactions, marine and laboratory chemistry have often little in common. This is due, in particular to the high degree of dissemination - down to « trace element » importance - of chemicals in the marine environment, to the active interplay between purely chemical and physico-chemical reactions (adsorption-desorption on particles, complexation, flocculation, sedimentation, resuspension, change of phase ... with simultaneous chemical transmutations) and to the intricate relationship between chemical and biological processes from bacterial activity to the translocations of chemicals through the food chain and their removal - with perhaps a carbon load of atmospheric CO₂ origin - in the shelf slope and deep sea sediments.

Marine ecosystems are the tuning-key of biogeochemical balances in the sea and a good understanding of the intensity and spatial patterns of marine productivity is necessary to appraise the (stabilizing ?) role of marine ecosystems in global changes of the environment. Ecosystem models are also necessary to assess the ecosystem's vulnerability to contaminants of anthropogenic origin and to calculate the transfer and accumulation of toxic substances from one level of the food web to the next. Marine biogeochemical models, the core of which is ecosystem dynamics, are generally speaking, time-dependent three-dimensional *active* transport-dispersion models with multiple interactions between the state variables requiring the simultaneous solution of several coupled evolution equations. For this reason, early ecosystem models have often been limited to box models, completely integrated over a whole region of the sea. One now realizes that spatial patterns of populations are essential features of ecology and environmental protection. Extending the model to two or three dimensions in space is not possible if, simultaneously, the scope of the model is enlarged, seeking a more and more detailed description of the ecosystems. For environmental studies, simple ecosystem models must be constructed. This can be done by taking advantage of their

natural **hierarchical organization** which results from the different rates of ecological processes confronted to a multi-scale physical environment (e.g. O'Neil 1989, Nihoul and Djenidi 1991). Processes with similar time scales constitute distinct levels in the hierarchy. Phenomena, on a particular level, are, to a large extent, dissociated from lower level « noise » or higher level « global trend » and may be relatively singled out of the total complexity of the ecosystem. Viewed through the appropriate « spectral window » (i.e. range of time scales and length scales) ecological processes can then be studied as comparatively simple systems.

One may consider ecological interactions at various levels : individuals, schools, populations ... with an overall range of temporal variability extending from fractions of seconds to several years. As pointed out before, however, a model cannot address all levels in a common deterministic description and attention must be restricted to one or the other dominant band of scales defining the spectral window of the model.

At the Globec Numerical Modelling Group Meeting in Nantes (Globec 1995), two main spectral windows have been identified, the first one, -associated with typical production rates -, corresponds to characteristic times from hours to days ; the second one, - associated with typical life times -, corresponds to characteristic times from weeks to months. The physical processes include, for the first window, diurnal variations of light and air-sea interactions, inertial oscillations, tides, storm surges and, for the second window mesoscale/synoptic eddies, frontal currents meandering and instabilities Larger frequencies (mesoscale and smallscale) processes such as internal waves, Langmuir cells and 3D turbulence are traditionally regarded as stirring mechanisms increasing the encounter rates between particles which themselves react passively to the physical forcing at those scales. There might be however, especially for zooplankton, some smallscale biological/physiological processes (related to the way of feeding, communicating or moving ...) the scales of which match the scale of the physics and one should consider the possibility of the existence of a third spectral window in the smallscale range.

State variables are defined by (i) their nature (e.g. phytoplankton, zooplankton ... biomasses), (ii) their spectral window i.e. the range of length scales and time scales under study (e.g. diurnal or seasonal variations ...). The number of state variables can be increased by refining the description on either of the two axes.

- (i) The **minimum critical set** contains a limited number of aggregated variables sufficient to reveal the cogent effects of the 3D time dependent physics on biological fields.
- (ii) The **optimum set** will contain all state variables necessary to describe the basic dynamics of the ecosystem, reproducing the correct energy budget (in the sense that additional state variables would not improve significantly the energetics).
- (iii) Although the optimum set is able to describe satisfactorily the dynamics of the ecosystem, it may not provide the answers to specific research questions. These may require additional state variables appropriate to each case and lead to **research sets** adapted to specific research objectives.
- (iv) Computational and intellectual limitations, the difficulty of interpreting too large sets of data, the increasing uncertainty on the values of parameters as their number increases faster than the number of state variables and the difficulty to collect enough data to initiate and operate large models, set a limit to the size of the set of state variables and one must expect that, at the present time, there is a **maximum size** of feasibility.

Coupled hydrodynamic/ecosystem models have benefited from the vast amount of research which has been devoted, separately, to the development of two-dimensional and three-dimensional hydrodynamic models, on the one side, of one-dimensional and box ecosystem models on the other side. While hydrodynamic models, rooted in a well-defined, non disputed, set of state variables, have progressively evolved towards a common standard form, applicable to both oceans and shallow coastal seas, with only slight differences in the formulation of turbulent closures or vertical stratification effects, ecosystem models, - limited as they are in the number of tractable variables and the necessity to restrict attention to those which best describe the specific system under study -, have diversified into a broad palette of sub-models which, despite a common philosophy and methodology, differ by the way of, economically, traducing in mathematical term the particulars of the problem.

A comparative listing of existing models (and their governing equations) would fall beyond the scope of this paper and would contribute little more than the excellent monographs, state of the art reviews and other syntheses which have been published over the years since the pioneer publications several decades ago. The following selection of

references is undoubtedly biased by their availability in the authors' library but the authors are confident that they, themselves, include enough references to allow the readers to reconstruct the whole web of relevant publications (e.g. Dugdale 1975, Steele 1975, 1985, Platt et al 1981, Wroblewski 1983, Parsons et al 1988, Walsh 1988, Longhurst 1989, Dugdale and Wilkerson 1989, Wada et al 1991, Lalli and Parsons 1993).

As pointed out before, the rates of production-destruction Q^y are not straightforward applications of chemical kinetics or ecology because environmental models describe the evolution of *aggregates* (particulate organic matter, plankton, ...) and the interactions contributing to Q^y are *translocations*, i.e. transferences in state space. These translocations must be parameterized in suitably close tractable forms which are inspired by - and respect - the laws of physico-chemistry and ecology but are not direct incarnations of them (e.g. Nihoul et al 1994, Delhez and Martin 1992, 1994).

Surprisingly good results are obtained by combinations of prey-predator kernels of the form $\alpha(\phi)z$ where ϕ is the prey and z the predator and where α is given by the Michaelis Menten kinetics.

$$\alpha(\phi) = \frac{c_1\phi}{c_2 + \phi}$$

or slightly modified versions of it.

This equation gives a linear relation for small $\phi(\phi \ll c_2)$ and tends to a constant for large $\phi(\phi \gg c_2)$.

For instance, if phytoplankton feeds on a nutrient n and is grazed by the zooplankton z , one would have

$$Q^\phi = \frac{a_1 n}{a_2 + n} \phi - \frac{c_1 \phi}{c_2 + \phi} z$$

a_1, a_2, c_1, c_2 being constants or functions of auxiliary variables (for instance light intensity, in the case of a_1).

The question however still remains whether expressions of this type, if valid in a certain range of scales, can be extended to other spectral windows (and if not what is their spectral domain of applicability?). This will require a careful reexamination of the formulation of the production/interaction rates and the development of time-nested

models, (i) run in typical conditions to provide the necessary guidance and/or (ii) interactively data-assimilated in the long range forecast.

3. Illustrative examples and applications

In this section, two examples of coupled 3D time-dependent models are presented and illustrated with applications. The objective here is not to single out one model rather than another, compare models or initiate a discussion on model validation, it is solely to display typical results of coupled models, to show the type of information these models can provide on the ecosystem space-time dynamics (even with a rather simple description of the ecosystem itself) and let the readers judge by themselves whether the product is worth the effort (or whether they would rather affect additional resources to the development of more sophisticated ecosystem box-models).

The Harvard Model

The Harvard dynamical model hierarchy is a flexible and portable regional-to-basin scale model set designed to be applicable to an arbitrary block of ocean. The domain boundaries may be partially or fully open or closed with realistically shaped coastlines and bottom topography. Extensions to coastal, shelf and shelf-break domains are well underway. The dynamical model options include primitive equations or quasigeostrophic dynamics throughout the water column with or without a coupled surface boundary model of the upper ocean. Other components of the Harvard forecast system are the statistical model set and the data analyses and management schemes. Data is mapped onto regular grids via (multivariate) objective analysis schemes which interpolate via the minimization of selected expected error norms. Additionally, statistical model components may include empirical orthogonal functions, in the horizontal or vertical, or other modal representations. Of special note are statistical model representations of typical synoptic structures, the feature models, which are utilized to minimize the observational data requirements necessary to achieve a synoptic realization of the state of the system. Analysis, initialization, and data assimilation schemes meld various types of data with different sampling schemes into estimates of field of interest, input data into models and produce melded estimates from observations and dynamical model output. Interdisciplinary extensions of the physical model system include acoustical and

biogeochemical/ecosystem models. A modular approach is used to develop an ecosystem model hierarchy, involving the study of biological and chemical processes first with the simplest biogeochemical/ecosystem model but with real ocean physical structures and extending the model if more complexity is necessary or interesting (e.g. Robinson 1993, 1994). The first study completed (Mc Gillicuddy 1993, Mc Gillicuddy et al 1995a,b) employed a 5-component model (phytoplankton, heterotrophs, nitrate, ammonium and exported nitrogen) to study the 1989 spring bloom in the Northeast Atlantic.

Some exemplary results are shown in figs. 2-4.

Fig. 2. shows the temporal development of the physical and biological fields. Day 115 is prebloom, 151 is end of bloom and 180 is postbloom. Three interacting eddies provide vertical nutrient transport into the euphotic zone that increases the nitrate by an order of magnitude over the background as shown in fig. 3. An actual ship-track of the field program overlying the simulated eddy field is shown by the solid line on the top of fig. 4 with corresponding along track mixed layer nitrate time series shown in the bottom of fig. 4. (The dashed track and time series is a simulated slight excursion of the ship which gives a simulated time series that agrees with the data everywhere).

The GHER Model

The three-dimensional ecohydrodynamic mathematical model developed at the **GeoHydrodynamics and Environment Research Laboratory (GHER)** of the University of Liège comprises a Primitive Equation dynamic model and a variational inverse model used in concerted - data assimilation liaised - operation (Nihoul and Djenidi 1987, Nihoul et al 1989, Nihoul 1993, Nihoul et al 1993, 1994). In its present form, the GHER Model consists in two sectorial submodels.

- i. the hydrodynamic model, the state variables of which are the three components of the velocity vector, the pressure, temperature, buoyancy (or salinity), the turbulent kinetic energy and the turbulent dissipation rate (or the mixing length) ;
- ii. the plankton ecosystem model, the state variables of which are the concentrations of nutrients (basically nitrate and ammonium), the biomasses of phytoplankton and zooplankton (describes as one or several size-separated aggregates), bacterioplankton and the concentrations of (particulate and dissolved, or total)

organic matter (interactions with the benthic ecosystem are treated in the bottom boundary conditions).

Figs. 5-10 show results of the application of the model to the summer general circulation and ecosystem dynamics in the Northern Bering Sea (Nihoul et al 1993, 1994).

Horizontal transport in the Northern Bering Sea is, to a large extent, determined by the inflow, deployment and outflow of the Anadyr Stream which penetrates the basin through the Anadyr Strait separating the Siberian peninsula from St. Lawrence Island. Strong upwelling/upsloping vertical motions are maintained along the Siberian coast by the passing of the stream (Ekman secondary flow enforced by strong vertical mixing). (figs. 5,6,7 and 8). Nutrient rich upwelled waters are entrained by the Anadyr Stream into the Northern Bering and Chukchi Seas. High phytoplankton biomasses are found in the frontal region where nutrient rich Anadyr waters and Alaskan waters meet and where frontal instabilities provide the conditions of enhanced photosynthesis (figs. 9 and 10).

Figs. 11-15 show results of the application of the model to the North Sea (Delhez and Martin 1992, 1994). The model predicts the beginning of the phytoplankton bloom in April in the well-mixed shallow Southern and coastal regions where it is further enhanced by important river inputs of nutrients (fig. 11). The prediction of the model is confirmed by the CZCS satellite image of Spring 1982 (fig. 12).

The bloom extends to the deeper waters in the North, later in the year, when the stratification is established and the depth of the mixed layer is reduced to, more or less, the thickness of the euphotic zone (figs. 13 and 14).

References

- Blumberg A.F. and Mellor G.L., (1985). A description of a three-dimensional coastal ocean circulation model. In : Three-dimensional Shelf Models, Coastal and Estuarine Dynamics, N. Heaps (ed.), American Geophysical Union, 5.
- Denman K.L. and Gargett A.E., (1983). Time and space scales of vertical mixing and advectons of phytoplankton in the upper ocean, *Limn. Oceanogr.*, **28** (5), 801-815.
- Denman K.L., (1994). Scale-determining biological-physical interactions in oceanic food webs, In : Aquatic Ecology : Scale, Pattern and Processes, P.S. Giller, A.G. Hildrew and D.G. Raffaelli (eds), 377-402.

- Delhez E. and Martin G., (1992). Preliminary results of a 3D baroclinic numerical model of the mesoscale and macroscale circulations on the North-Western European Continental Shelf, *Journal of Marine Systems*, **3**, 423-440.
- Delhez E. and Martin G., (1994). 3D modelling of hydrodynamic and ecohydrodynamic processes on the North-Western European Continental Shelf, *Bulletin de la Société Royale des Sciences de Liège*, **63**, 5-64.
- Denman K.L. and Powell T.M., (1984). Effects of physical processes on planktonic ecosystems in the coastal ocean, *Oceanogr. Mar. Biol. Ann. Rev.*, **22**, 125-168.
- Denman K.L., Freeland H.J. and Mackas D.L., (1989). Comparisons of time scales for biomass transfer up the marine food web and coastal transport processes, *Can. Spec. Publ. Fish. Aquatic Sci.*, **108**, 255-264.
- Dugdale R.C., (1975). Biological Modelling I, In : *Modelling of Marine Systems*, J.C.J. Nihoul (ed.), Elsevier Publ., Amsterdam, 187-206.
- Dugdale R.C. and Wilkerson F.P., (1989). Regional perspectives in global new production, In : *Océanologie*, M. Denis (ed.), Centre d'Océanologie de Marseille, 289-308.
- Globec, (1988). Global ocean ecosystems dynamics, Report of a Workshop held at Wintergreen, Virginia, May 1988, V. Cullen (ed.), Joint Oceanographic Institutions Inc. Publ., Washington, USA, 131 pp.
- Globec, (1993). Proc. Meeting of the Numerical Modelling Group, Villefranche, France, July 1993.
- Globec, (1995). Proc. Meeting of the Numerical Modeling Group, Nantes, France, July, 1995.
- Horne J.K. and Schneider D.C., (1994). Analysis of scale-dependent processes with dimensionless ratios, *Oikos*, **70**, 201-211.
- Lalli C.M. and Parsons T.H., (1993). *Biological Oceanography*, Pergamon Press, Oxford, 301 pp.
- Longhurst A.R., (1989). Pelagic ecology : definition of pathways for material and energy flux, In : *Océanologie*, M. Denis (ed.), Centre d'Océanologie de Marseille, 263-288.
- Lumley J.L., (1978). Computational modelling of turbulent flow, *Advances in Applied Mechanics*, C.S. Yih (ed.), Academic Press, **18**, 123-176.
- Mc Gillicuddy D., (1993). Mesoscale ocean dynamics and biological productivity, Ph.D. Thesis, Harvard University, Cambridge, USA.
- Mc Gillicuddy D.J., Mc Carthy J.J. and Robinson A.R., (1995a). Coupled physical and biological modeling of the spring bloom in the North Atlantic. (I) : model formulation and one-dimensional bloom process, *Deep-Sea Research I*, **42**, 1313-1357.
- Mc Gillicuddy D.J., Robinson A.R. and Mc Carthy J.J., (1995b). Coupled physical and biological modeling of the spring bloom in the North Atlantic. (II) : three-dimensional bloom and post-bloom processes, *Deep-Sea Research Research I*, **42**, 1359-1398.
- Monin A.S., Kamenkovich V.M. and Kort V.G., (1977). *Variability of the Oceans*, J. Wiley & Sons, New York, 24 pp.
- Monin A.S. and Ozmidov R.V., (1985). *Turbulence in the Ocean*, D. Reidel Publ. Co., Dordrecht, 247 pp.
- Nihoul J.C.J., (1975). *Modelling of Marine Systems*, Elsevier Publ. Co., Amsterdam, 272 pp.

- Nihoul J.C.J., (1980). *Marine Turbulence*, Elsevier Publ. Co., Amsterdam, 378 pp.
- Nihoul J.C.J., (1984). A three-dimensional marine circulation model in a remote sensing perspective, *Annales Geophysicae*, **2**, 433-442.
- Nihoul J.C.J. and Djenidi S., (1987). Perspective in three-dimensional modelling of the marine system, In : *Three-Dimensional Models of Marine and Estuarine Dynamics*, J.C.J. Nihoul & B.M. Jamart (eds), Elsevier Publ. Co., Amsterdam, 1-33.
- Nihoul J.C.J., Deleersnijder E. and Djenidi S., (1989). Modelling the general circulation of shelf seas by 3D k - ϵ models, *Earth Science Reviews*, **26**, 163-189.
- Nihoul J.C.J., Djenidi S. and Hecq J.H., (1989). Modelling of coastal/shelf systems with emphasis on long term trends, *Int. J. for Num. Meth. in Eng.*, **27**, 113-127.
- Nihoul J.C.J. and Djenidi S., (1991). Hierarchy and scales in marine ecohydrodynamics, *Earth Science Reviews*, **31**, 255-277.
- Nihoul J.C.J., (1993). Applications of mathematical modelling to the marine environment, In : *Environmental Modeling*, vol. I, P. Zannetti (ed.), Computational Mechanics Publ., Southampton, 75-140.
- Nihoul J.C.J., Adam P., Brasseur P., Deleersnijder E., Djenidi S. & Haus J., (1993). Three-dimensional general circulation model of the Northern Bering Sea's summer ecohydrodynamics, *Continental Shelf Research*, **13**, 509-542.
- Nihoul J.C.J., Adam P. and Brasseur P., (1994). Mathematical visualisation of the Northern Bering Sea's summer ecohydrodynamics. In : *Data Assimilation : Tools for Modelling the Ocean in a Global Change Perspective*, Brasseur P. & Nihoul J.C.J., (eds), NATO ASI Series, Springer Verlag, vol. **119**, 239 pp.
- O'Neill R.V., (1989). Perspectives in hierarchy and scales, In : *Perspectives in Ecological Theory*, J. Roughgarden, R.M. May & S.A. Levin (eds), Princeton University Press, Princeton, N.J., USA, 140-156.
- Parsons T.R., Takahashi M. and Hargrave B., (1988). *Biological Oceanographic Processes*, Pergamon Press, Oxford, 330 pp.
- Platt T., Mann K.H. and Ulanovicz R.E., (1981). *Mathematical models in biological oceanography*, The Unesco Press, Paris, 156 pp.
- Robinson A.R., (1993). Physical processes, field estimations and interdisciplinary ocean modeling, In : *Numerical Modeling*, Globec Report Series **6**, Globec International Ed., Solomons, USA, 45-52.
- Robinson A.R., (1994). Predicting and monitoring of the physical-biological-chemical ocean, *Globec Special Contributions 1*, Globec International Ed., Solomons, USA, 23 pp.
- Rodi W., (1985). Survey of calculation methods for flow and mixing in stratified fluids. In : *Proceedings IUTAM Symposium on Mixing in Stratified Fluids*, Margaret River Western Australia, August 1985, 1-51.
- Steele J.H., (1975). Biological Modelling II, In : *Modelling of Marine Systems*, J.C.J. Nihoul (ed.), Elsevier Publ., Amsterdam, 207-216.
- Steele J.H., (1985). A comparison of terrestrial and marine ecological systems, *Nature*, **313**, 355-358.
- Wada E. and Hattori A., (1991). *Nitrogen in the Sea : Forms, Abundances and Rate Processes*, CRC Press, Boston, 208 pp.
- Walsh J.J., (1988). *On the Nature of Continental Shelf*, Academic Press, San Diego, 520 pp.
- Wroblewski J.S., (1983). The role of modeling in biological oceanography, *Ocean Science and Engineering* **8**, 245-285.

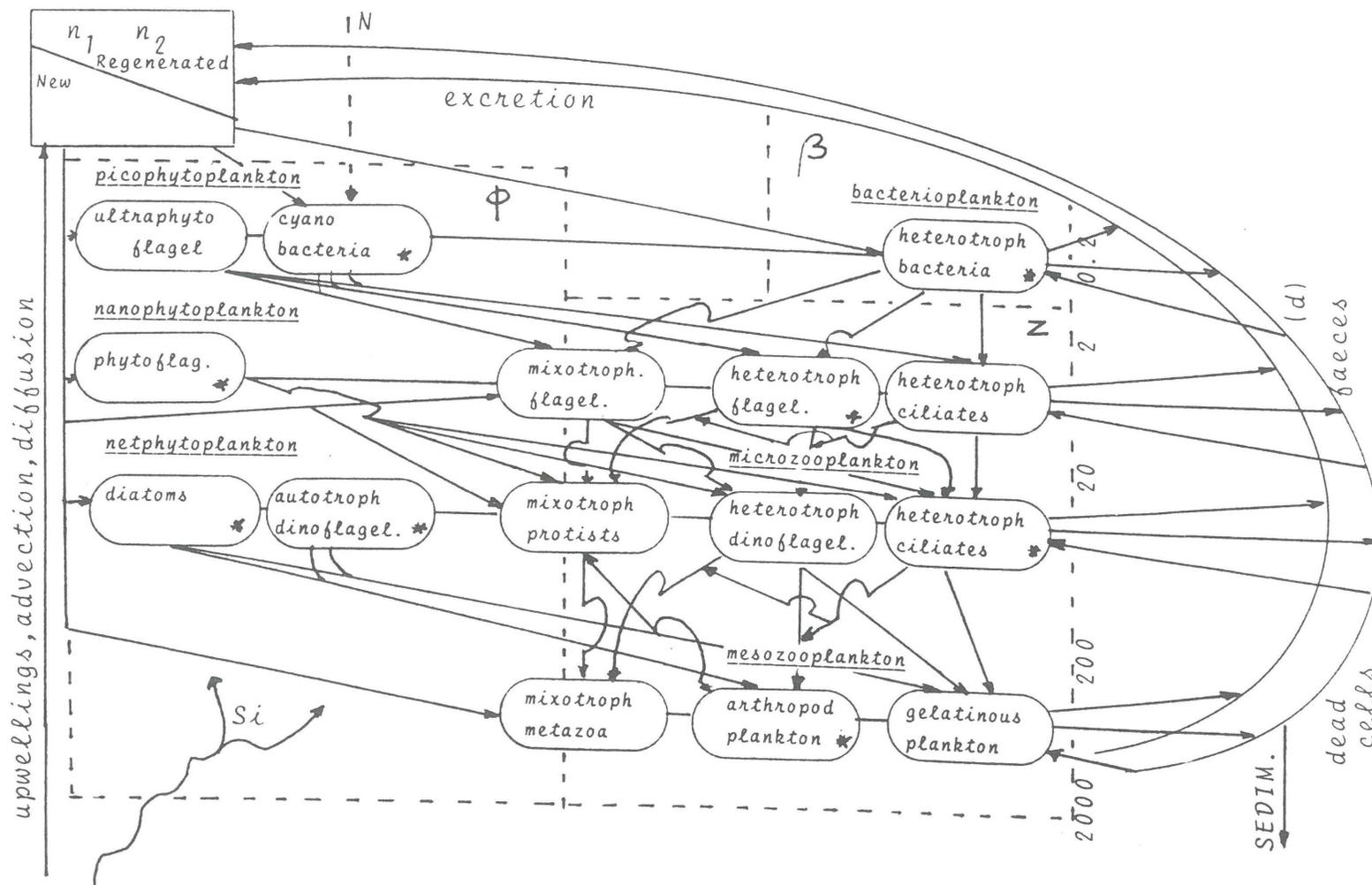


Fig. 1 : Plymouth NATO ASI consensus food web model 1988.
 * aggregates in Fenchel's model ;
 underlined are the aggregates in the model of Moloney and Field.

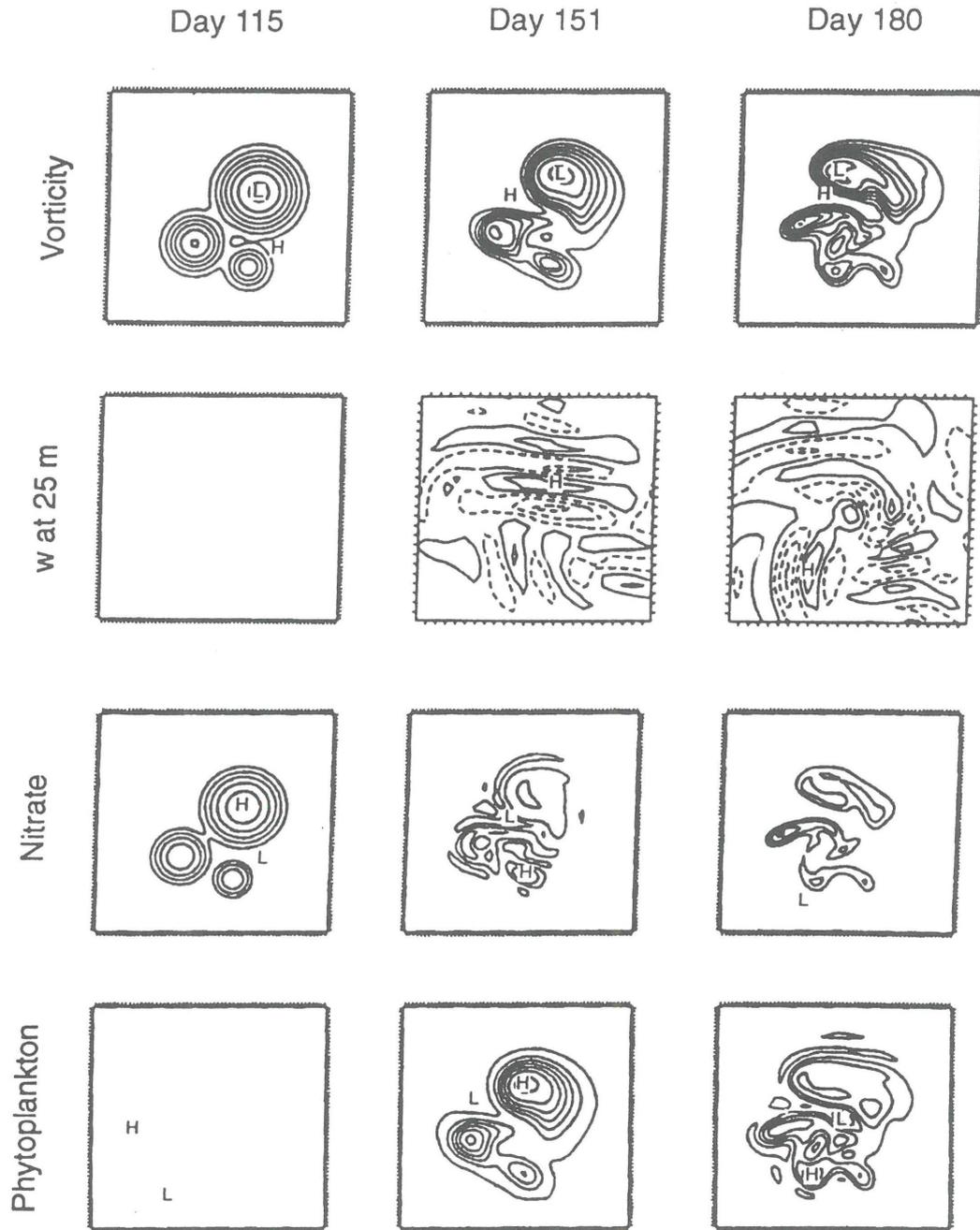


Fig. 2 : Temporal development of physical and biological fields. Day 115 is prebloom, 151 is end of bloom and 180 is postbloom. See Mc Gillicuddy (1993) for details.

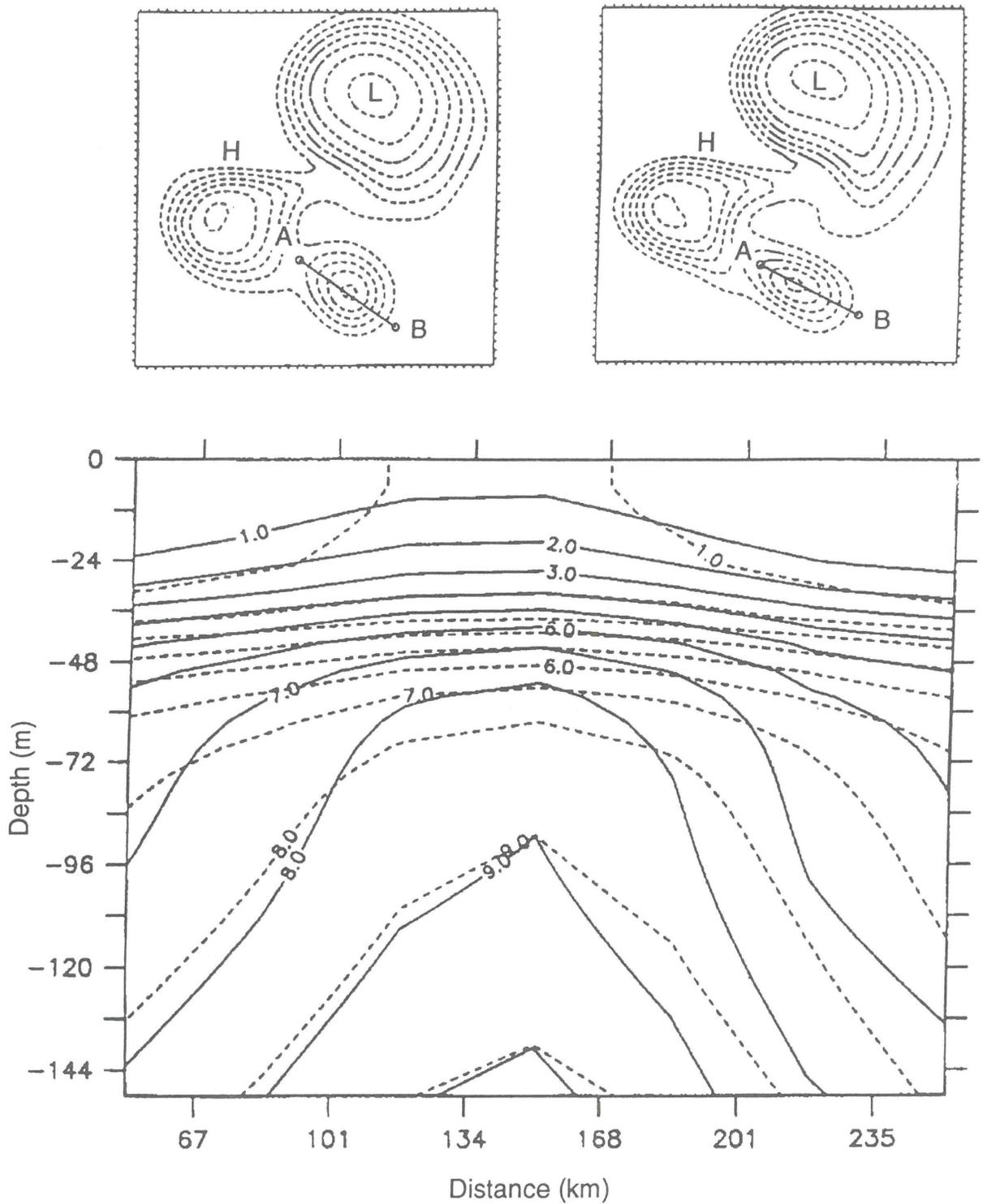


Fig. 3 : Maps of non-dimensional top density on day 139 (left above) ; day 151 (right above).
Below : vertical section of nitrate taken from A to B on day 151 (dashed contours) overlaid on the section taken on day 139 (solid contours).

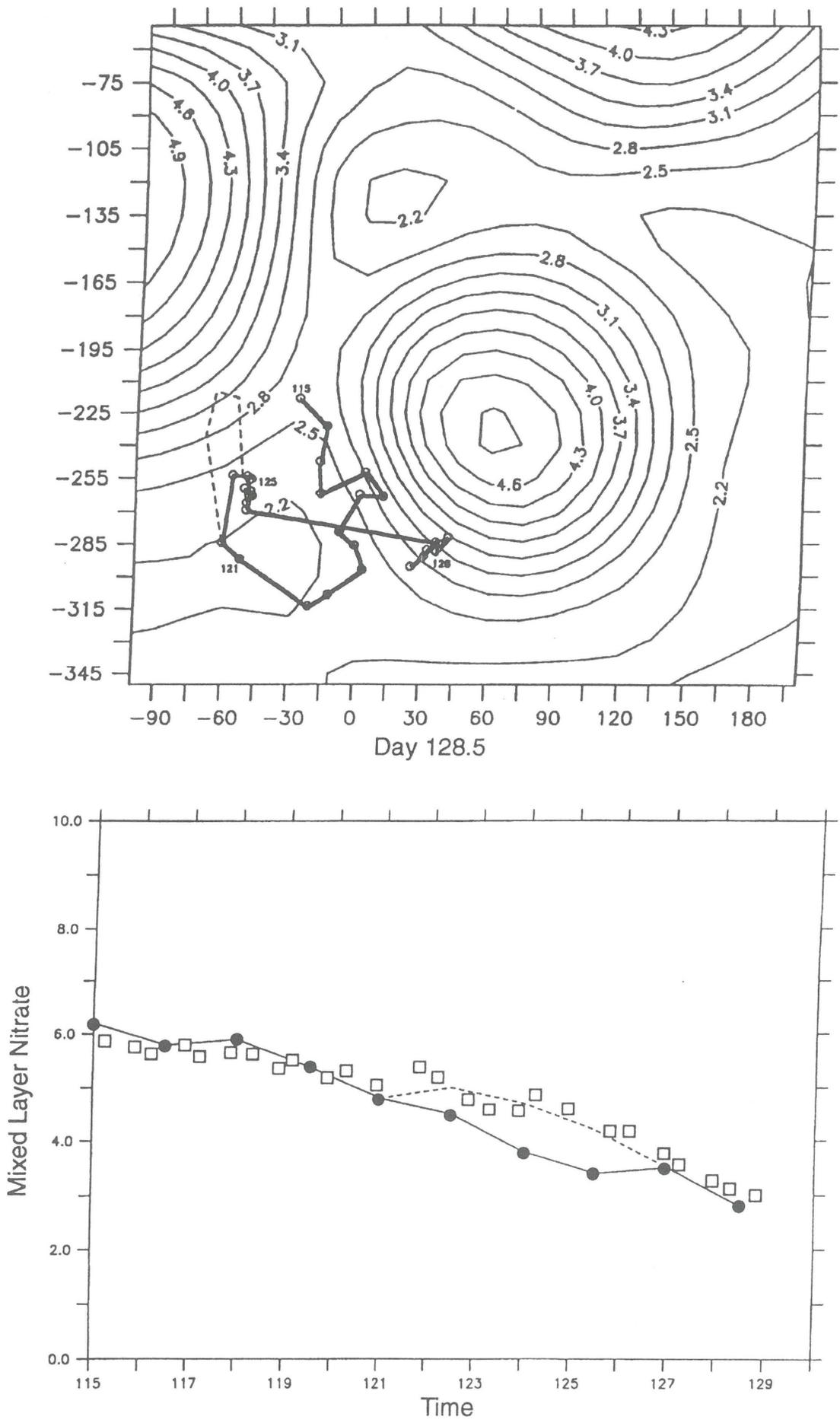


Fig. 4. : a) The actual (solid line connecting open circles) and hypothetical (dashed line) cruise track overlaid on a map of mixed layer nitrate concentration on day 128 of the three eddy simulation. b) Mixed layer nitrate concentration observations (squares) and values extracted from model along the actual (solid line) and the simulated (dashed line) cruise track.

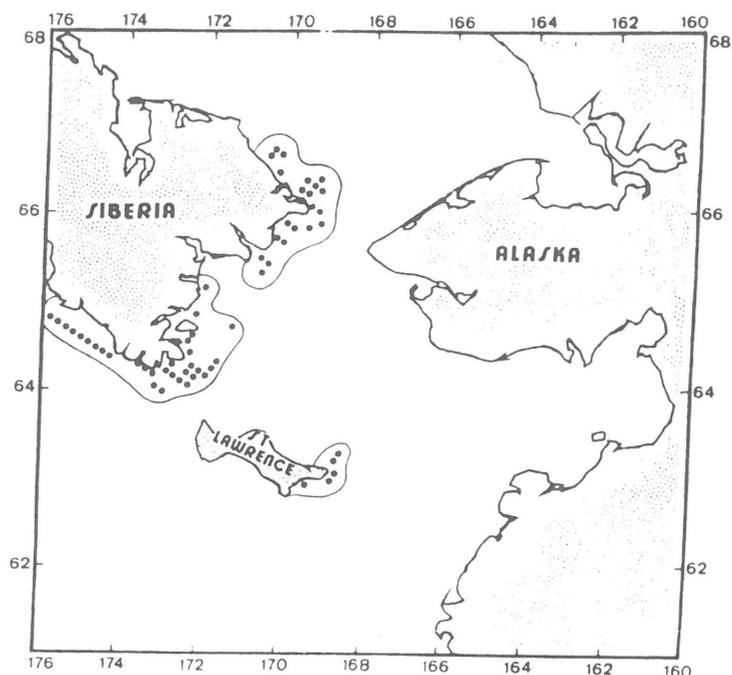


Fig. 5. : Upwellings/up-sloping along the Siberian coast and the East coast of St. Lawrence Island indicated by grid points where the upwelling/up-sloping vertical velocity is significantly high (as much as 4 m day^{-1} on the western side of the Anadyr Strait) (reference summer situation).

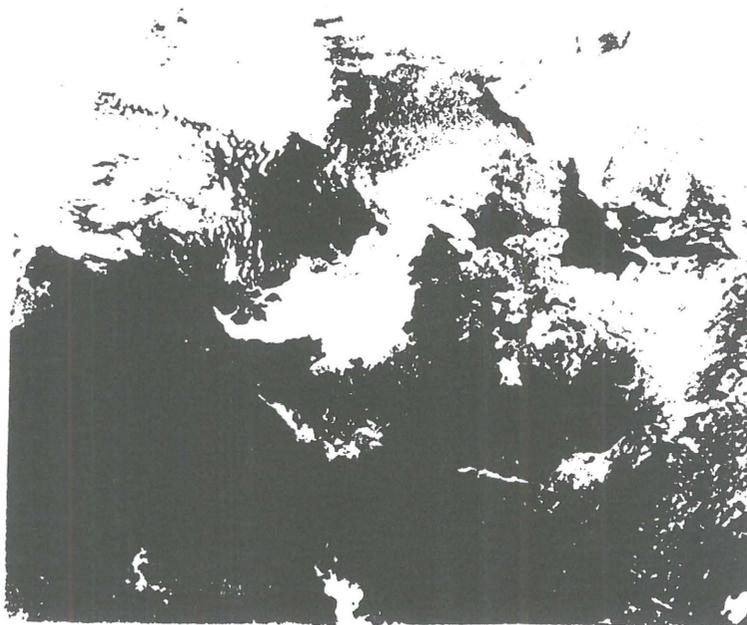


Fig. 6. : Remote sensing photograph of the northern Bering Sea (27 August 1987) showing the upwelling and cold plume of nutrient rich water coming upon along the Siberian coasts in the Strait of Anadyr and spreading northwards and eastwards under the action of the currents, with additional interleaving layers flowing to the east.

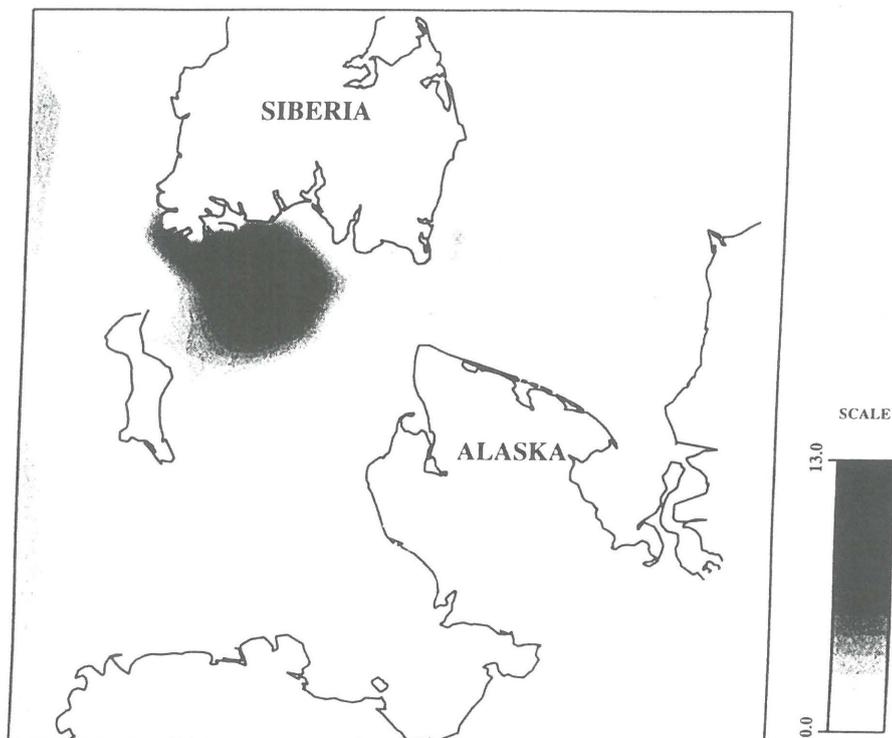


Fig. 7. : Surface distribution of nitrate ($\text{mg} \cdot \text{atNm}^{-3}$).
Reference summer situation computed by the mathematical model.

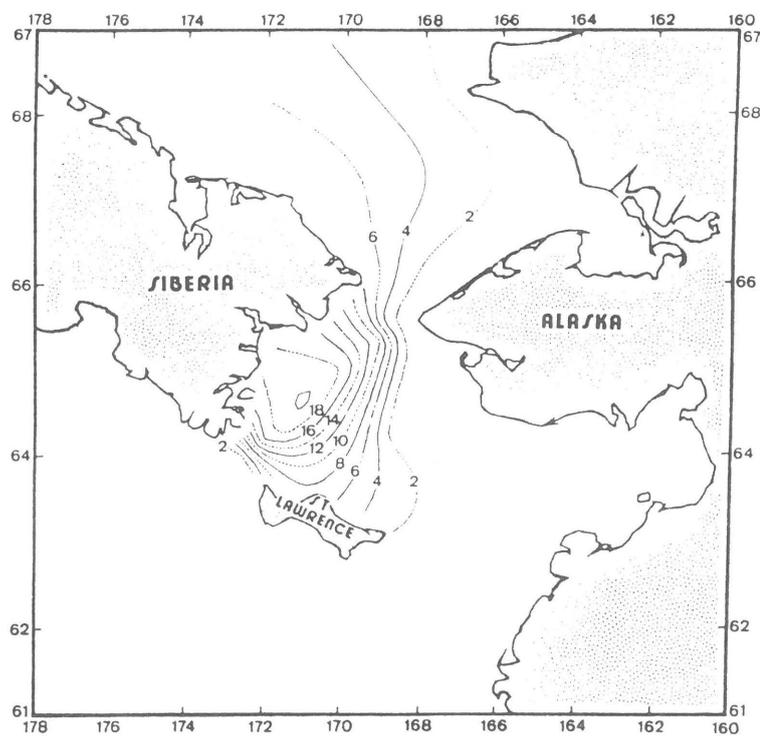


Fig. 8. : Surface distribution of nitrate reconstructed by the Variational Inverse Model
from the data of cruise HX71 ($\text{mg} \cdot \text{atNm}^{-3}$).

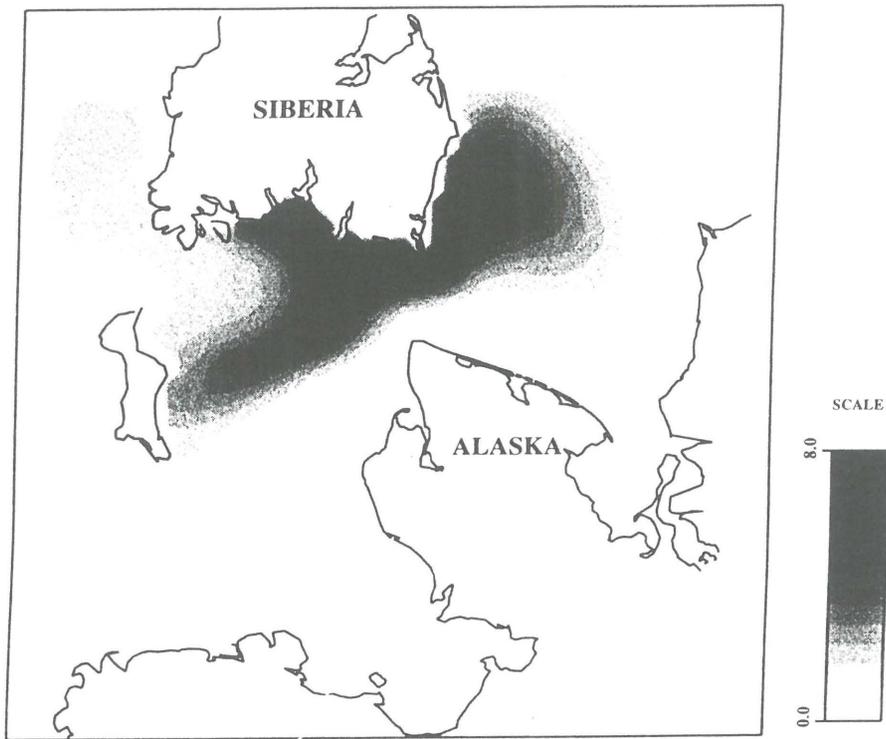


Fig. 9. : Surface distribution of phytoplankton ($\text{mg} \cdot \text{atNm}^{-3}$).
Reference summer situation computed by the mathematical model.

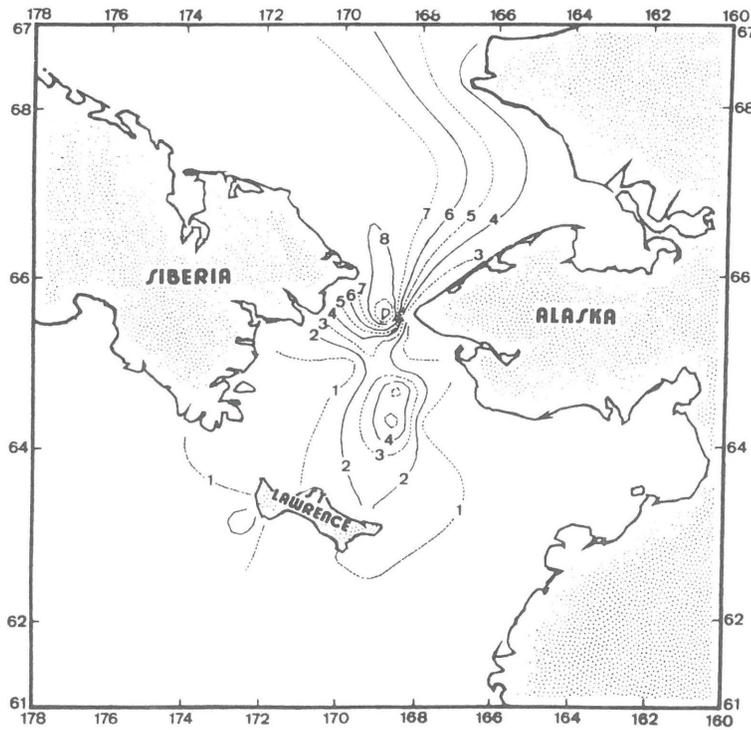


Fig. 10. : Surface distribution of chlorophyll a reconstructed by the Variational Inverse Model from the data of cruise HX71 ($\text{mg} \cdot \text{atNm}^{-3}$).

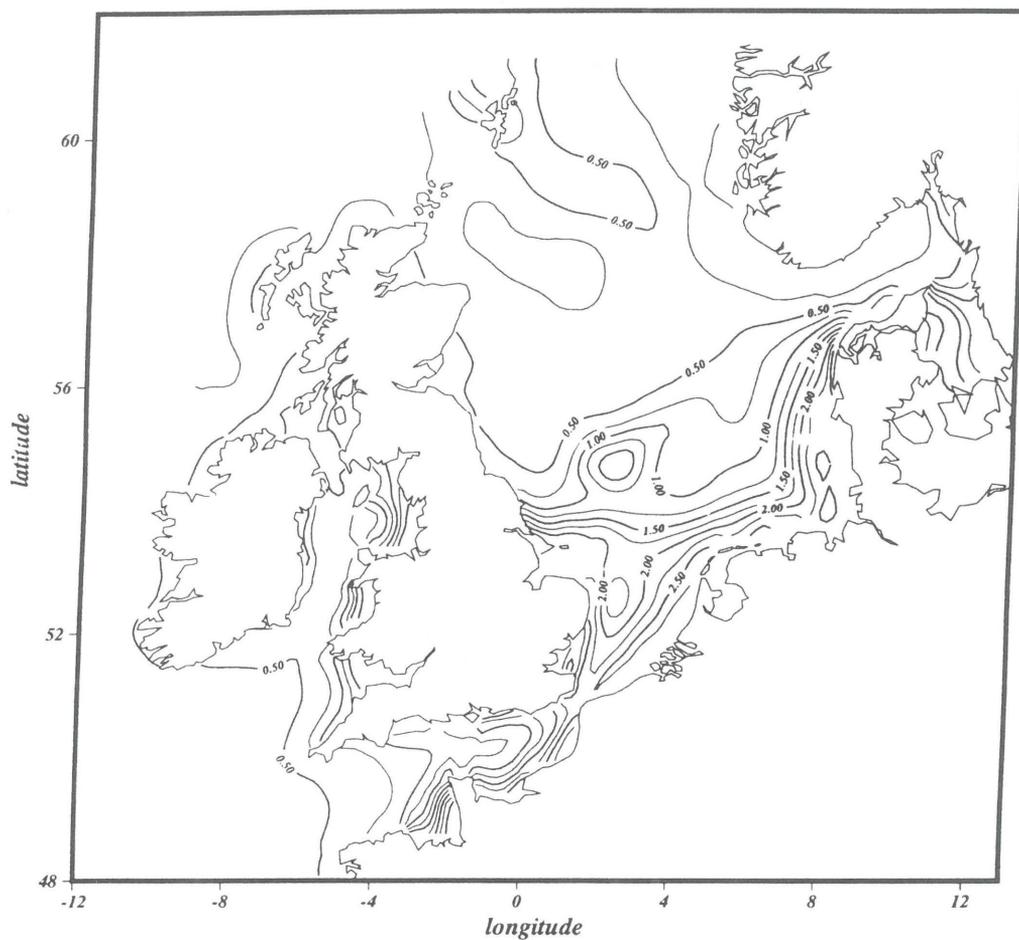


Fig. 11. : Beginning of phytoplankton bloom in the well-mixed shallow southern and coastal regions of the North Sea, in early spring (Isolines of surface chlorophyll concentrations in mgChlam^{-3}).

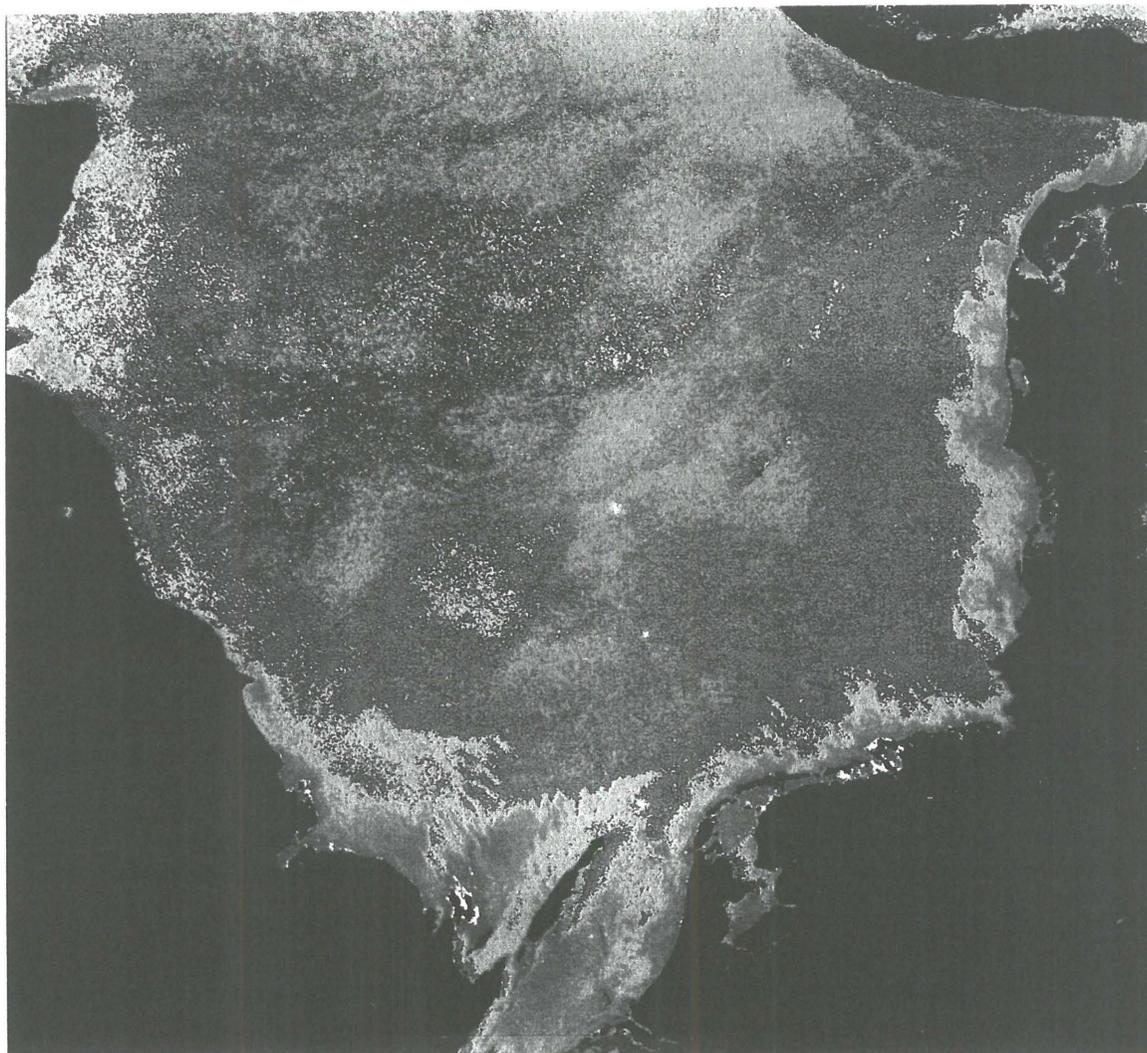
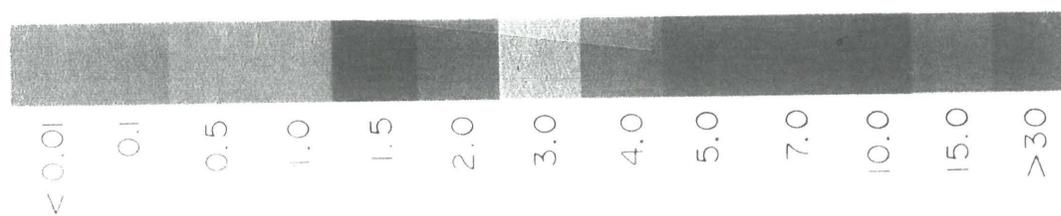


Fig. 12. : CZCS Satellite image of phytoplankton distribution in early spring in the North Sea.



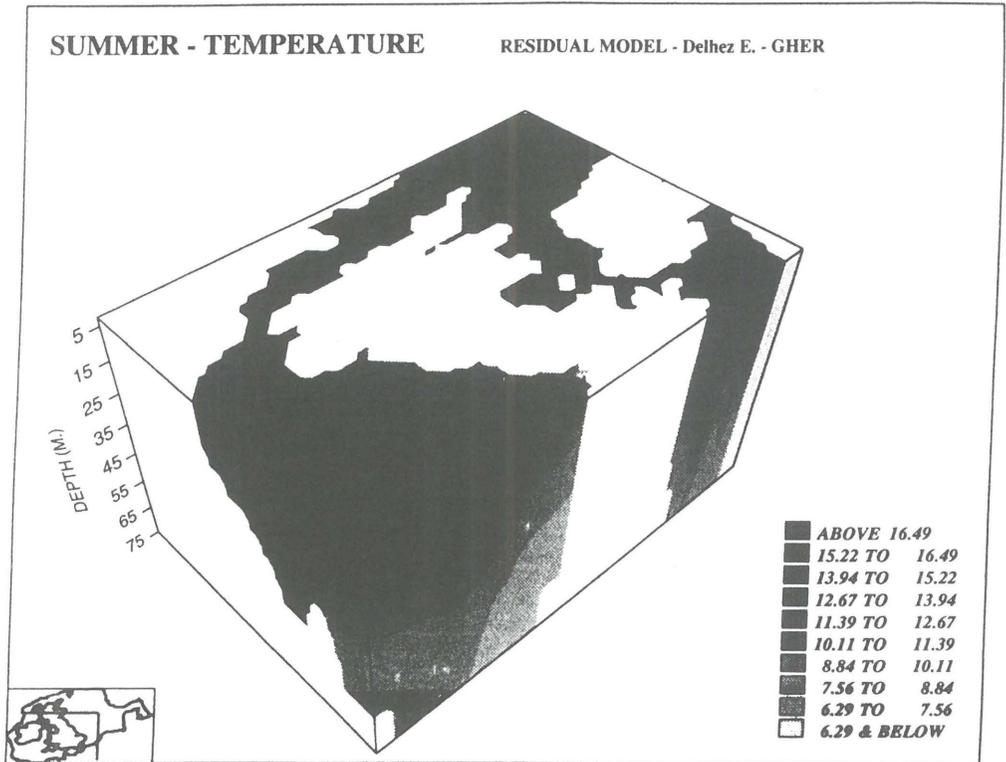


Fig. 13. : Three-dimensional view of the summer temperature in the North Sea seen from the North East showing the stratification in the deep central part and well-mixed conditions in the shallow Southern Bight.

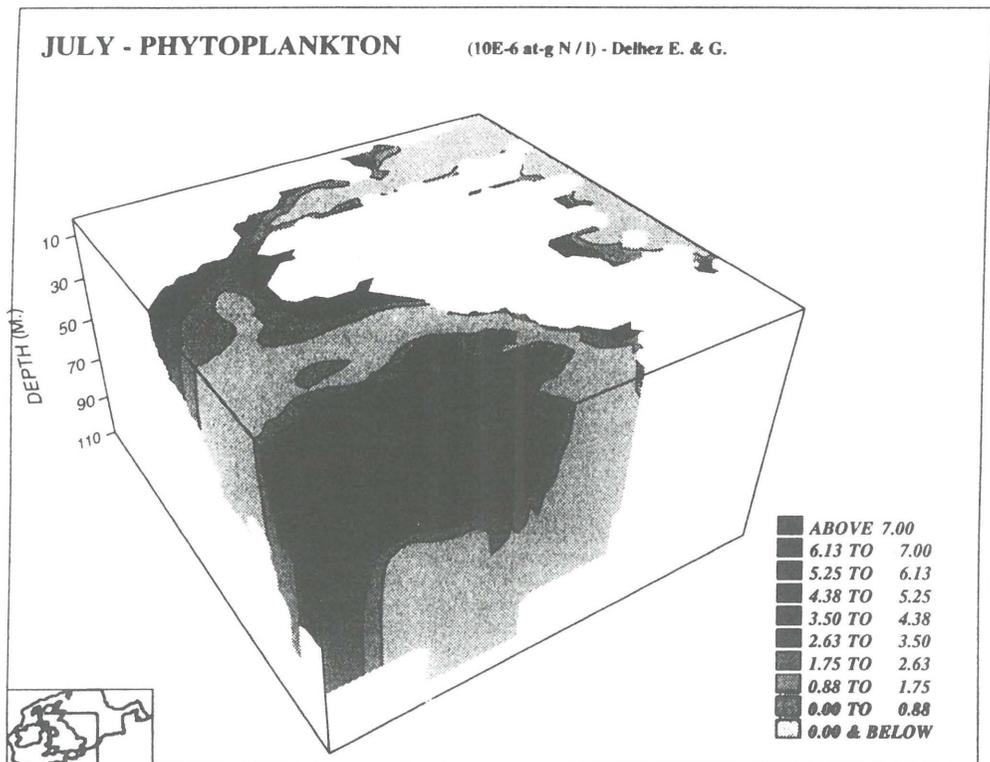


Fig. 14. : Three-dimensional view of the summer phytoplankton distribution seen from the North East as in fig. 12 showing the primary production in the stratified central part.

