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Towards Water Quality Models [and Discussion]

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Towards water quality models

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[Plates 1 and 2]

Predictions of water quality involve the modelling both of physical processes, which underlie the transport and diffusion of all constituents, and of the sources, sinks, partitioning and interactive processes individual to those constituents. These processes are outlined, together with complementary modelling approaches: (i) development of sophisticated three-dimensional models to represent the physics, and sub-models of suspended sediment, microbiology and metal interactions for processes controlling nutrients, dissolved oxygen, phytoplankton, detritus and metals; (ii) a framework to link these component models; (iii) an accessible model with simpler physics for wide use in simulating constituent distributions, for comparison with measurements to infer sources, sinks and interactions. The North Sea Project measurements provide an input in process evaluation, and data to test the models.

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1. Introduction

Models for water quality have many purposes: aiding experimental design; linking cause and effect, e.g. through model experiments; running different scenarios for hypothetical questions; predicting evolution of constituent fields through time (Huthnance 1988). These research and management or policy interests all need accurate prognostic models, predicting states at future times from an initial state.

A common approach to prediction applies for many water-quality constituents, be they dissolved, particulate, in the biota, suspended sediment or adsorbed thereon. For any one constituent and phase in a conceptual 'box' anywhere in the mobile marine environment (sea surface, interior, coastal or bottom boundary, or in the sediment),

'Prognostic' rate of change = influx (through advection, settling, mixing)
+ sources − sinks (including phase transfers).

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The sources and sinks are governed by chemical, biological or sedimentological processes specific to the individual constituent and phase. However, physics common to all constituents determines the influx contributions and provides the spatial and temporal context of this advection–diffusion equation.

A numerical formulation tends to be necessitated by the complex spatial domain, by the many equations for the various constituents and phases, and by these equations' nonlinearities in the flux terms and source-sink processes coupling the constituents and phases. This paper's theme is progress towards coupled models of such processes.

(a) *Processes*

Sediments play a key role and exemplify process coupling. In shallow waters, with strong wave-enhanced stresses from near-bed currents, suspended sediment absorbs light and so limits photosynthesis. These stresses can also release contaminants from pore-waters of cohesive sediments. Metals introduced into coastal waters and the ocean may be transported on particle surfaces as well as in solution; the timescales of metal sorption processes are influenced by particle type (e.g. biogenic or inorganic). These factors determine whether metals are deposited on the shelf with settling particles or advected to the open ocean; the understanding of particle–water interactions is central to modelling the behaviour of these elements, and similarly for organic pollutants.

Organic aspects of marine water quality are associated with the activity of microorganisms, especially the rapid light-driven synthesis of organic material and its slower mineralization. With seasonal stratification, photosynthesis dominates towards the sea surface and mineralization in deeper water and the benthos. In shallow, tidally stirred, waters the two groups of processes co-exist in a single mixed layer that contains much suspended sediment.

Plankton growth is controlled by the availability of light energy and of the so-called nutrient elements (nitrogen, phosphorus and silicon). Available nutrients derive from (i) new supply to the system, e.g. from rivers, and (ii) return into solution (some via sediments) by remineralization. Human activities have increased the level of dissolved nitrogen and phosphorus above natural levels in rivers; the marine impact is an important water-quality question.

The dissolved oxygen concentration of marine and fresh water can be used as a sensitive indicator of water quality. Excess organic material from natural or anthropogenic sources imposes an elevated biological oxygen demand (BOD). Under particularly high organic loading, as can occur in some polluted North Sea estuaries such as the Schelde (Billen *et al.* 1988), or when reaeration of waters is prevented, as beneath the Baltic pycnocline (Stigebrandt & Wulff 1987), the waters become undersaturated with oxygen, or even anoxic. Such reduced-oxygen environments impose a physiological stress on the natural marine populations. Seasonal thermohaline stratification of the northern North Sea has caused low-oxygen waters to develop with ensuing benthos mortality, as well as phase changes for redox-sensitive metals.

(b) *Current status of water quality models*

The problem of developing a proven model to predict the fate of contaminants in shallow seas has been considered in GESAMP (1991) which reviews the processes to be included. Bewers *et al.* (1992) give the major findings, the scientific questions to be answered and the conceptual model developed.

Oxygen has been modelled in the context of estuarine water quality (e.g. Billen *et al*. 1988) and in the Baltic (Stigebrandt & Wulff 1987, with nutrients and using a physical–biochemical one-dimensional model to simulate seasonal changes in vertical profiles). Ecological modelling of the North Sea has been reviewed by Fransz *et al*. (1991).

The prediction of the fate of contaminants in the Dutch Coastal zone, the North Sea (GESAMP 1991) and macrotidal estuaries (van Eck & de Rooij 1990) is being achieved via the development of coupled models. A basic water and sediment transport module can be interfaced with other modules describing chemical and biological processes. The combined codes can determine (e.g.) dissolved and particulate nutrients and organic carbon, O_2, chlorophyll, pH, Eh, BOD and chemical oxygen demand, thereby integrating the roles of nutrients, primary productivity and dissolved oxygen. In addition, the chemical module is used for determining the concentrations and speciation of dissolved constituents, based on thermodynamics, and their surface complexation with particulate matter, incorporating the distribution coefficient (K_d). For some species the kinetics of sorption processes can be modelled. The object is to predict the concentrations of toxins in selected organisms.

(*c*) *Outline*

In this paper, we consider the modelling requirements and progress for groups of variables in turn. Physics (§2) comprises advective velocities, turbulent mixing, temperature and salinity, followed by suspended sediments. Nutrients, oxygen and microbiology (plankton, detritus) are considered together (§3) and finally metals (§4). Thus our scope is restricted to the lowest level of the food chain and quasi-continuum variables; reproductive discontinuities and transfers by larger animals generally demand a different approach.

Variables might be calculated in the sequence of §§2–4, neglecting reverse effects. However, a 'framework' (§5) allows their interaction; the use of a 'user-friendly' physics model to encourage parallel development for different constituents is also discussed.

2. Physics

For all constituents, advection is effected by the model-resolved velocity field. Full resolution implies three-dimensions (3D) (velocity decreases to zero at the sea floor and horizontal variations contribute to dispersion) and interactive inclusion of tidal, wind-driven and density-driven currents. *Tides* are often the largest currents in the North Sea (Huthnance 1991) and so control the level of friction and turbulence. Nonlinear advection and friction induce time-averaged tidal 'residuals' near short-scale topography or in the presence of internal tides, entailing model resolution to *ca*. 1 km. *Wind-driven* flow may be more sheared, especially across any seasonal thermocline, and movements in storms are known to be important compared with the mean circulation; models need 'actual' time-dependent winds and atmospheric pressure forcing. Evolving *density-driven* flow entails fine resolution corresponding to the Rossby radius of internal deformation, typically 1–5 km. Examples are fronts (Hill *et al*., this symposium), associated baroclinic eddies, and freshwater outflows as from the Rhine (Simpson *et al*. 1993).

'Mixing' should represent (parametrically) all unresolved aspects of the flow, especially in the near-field of any concentrations (Prandle *et al*., this symposium). Contributions necessarily include turbulence, and any of the above flows which are not modelled explicitly. (Transfer of momentum by these small scale processes also influences the large-scale flow.) The representation is usually either as a diffusion coefficient, parametrized or based more fundamentally on an explicit calculation of turbulence statistics, or by the addition of random displacements when a particle-tracking method is used, usually for sediments or non-physical constituents (e.g. Sündermann, this symposium). *Vertical* 'mixing' is known to depend on shear, stratification, tidal friction, winds and waves (e.g. Jago *et al.*, this symposium). *Horizontal* 'mixing' depends strongly on the model grid scale, according to the flow contributions which are not resolved explicitly, notably tidal shear dispersion; other contributions are discussed in Zimmerman (1986). Estimates of horizontal diffusion coefficients range from *ca.* 1 $m^2\,s^{-1}$ on scales 0.1–1 km (experimentally; see Elliott (1986) for oil droplets; Riepma 1985) to *ca.* 100 $m^2\,s^{-1}$ (Humber plume model with a 5 km grid, §3, empirically to match observed dispersion; elsewhere off coasts (Howarth *et al.*, this symposium)) and 300 $m^2\,s^{-1}$ (Prandle 1984; 35 km grid, also empirically). Special contexts may enhance values, e.g. 200 $m^2\,s^{-1}$ for circulation over sandbanks (theory; Zimmerman 1986), 400/80 $m^2\,s^{-1}$ along/across fronts on a 5 km scale (experiment; Durazo *et al.* 1993).

Turbulence and bottom stress affect both the flow and the suspension and movement of sediments (whose added density and particle dynamics introduce a distinct diffusivity). They need accurate representation in any 3D model (e.g. by turbulence closure methods as in Davies & Jones (1991)). Like vertical mixing, the turbulence and stress arise from shear (e.g. across the thermocline), imposed forcing, wind-wave breaking and flow over a rough sea bed. They are damped by stratification, even where this is due to the bed stress producing a large near-bed sediment load (Huntley *et al.*, this symposium). For a review, see Davies (1990). Enhancements in bed stress due to wind and wave turbulence in shallow regions can influence near-bed currents during major events. Such bed stress in models has to be parametrized (Grant & Madsen 1986) failing resolution of the wind–wave spectrum.

Temperature and *salinity* prediction is needed to force evolving density currents (fronts, eddies thereon, internal waves) and in view of substantial inter-annual variability (Howarth *et al.*, this symposium). They are themselves water-quality variables, relatively easily and accurately measured with different diffusivities and sources, and hence suitable as tests of models.

Appropriate open boundary conditions (e.g. Røed & Cooper 1986) tend to be model-dependent. For the present work, sufficient conditions have been (i) at the open-sea boundary, a radiational condition for elevations and currents additional to the prescribed tide, climatological temperature and salinity as appropriate; (ii) at the land boundary, zero normal flux plus freshwater input; (iii) atmospheric rainfall and evaporation; heating through bulk formulae (Lane 1989) according to wind, air and sea temperatures, cloudiness, etc.

A sequence of models has addressed these physical aspects. To provide a first estimate of the circulation during the 15-month survey period of the North Sea Project (NSP) use was made of hourly depth-averaged tide and surge currents and elevations from the U.K. operational storm surge model. Accuracy was checked by comparing modelled and observed U.K. surge elevations and by comparison of the modelled currents with mid-depth observations at the NSP moorings (Proctor & Smith 1991). The depth-averaged model circulation provides a good first-order estimate in the shallow well-mixed southern bight of the North Sea. In the northern North Sea, discrepancies occurs in summer; stratification there is not included in the

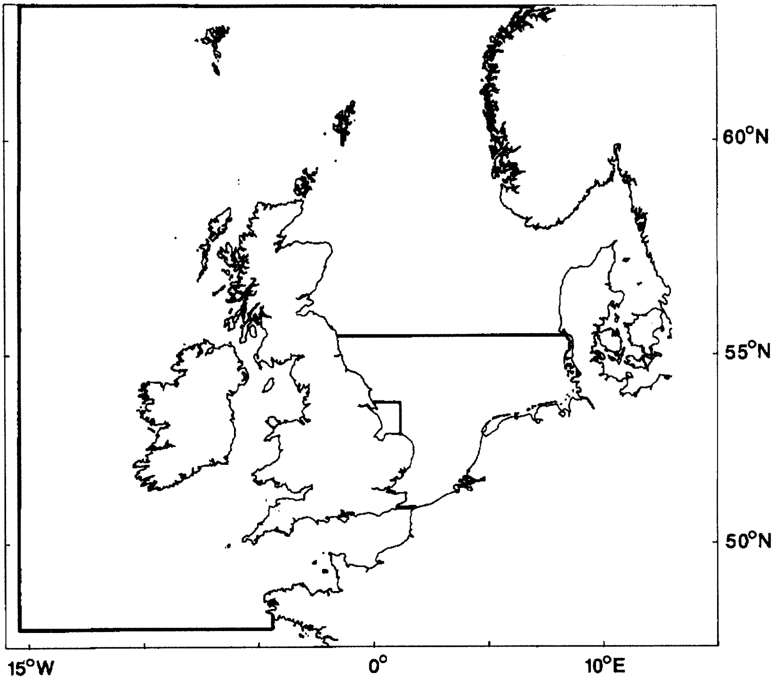

Figure 1. Chart of North Sea model areas. Outermost: 3D 15-month integration with diagnostic density; 1/5° × 1/3° grid. Intermediate: Dover Strait to $55\frac{1}{2}$° N. Innermost: Humber plume budgets.

model formulation. The daily mean circulation was the basis for interpreting (e.g.) nutrients and suspended sediment measured during the survey period (see below and Howarth *et al.*, this symposium).

For turbulence intensities varying through the tidal current cycle, 3D homogeneous models of the North Sea using turbulence energy closure schemes and resolving the high-shear bottom-boundary layer have proved successful (Davies & Jones 1991).

Effects of seasonal stratification have been included by running a 3D model (figure 1) for hourly elevation and current distributions throughout the 15-month NSP survey period. Adapted from Backhaus & Hainbucher (1987) the model incorporated climatic monthly-mean temperature and salinity distributions adjusted for observed anomalies. The diagnostic density distribution was varied daily as a linear interpolation of the monthly values. The resulting vertical stratification is more diffuse than observed, but the effect of the seasonal heating cycle is introduced. Tidal and meteorological forcing were included (surface winds and atmospheric pressure at 3 h intervals). Currents from this model give improved correlation with the NSP mooring measurements at all times of the year.

Towards prognostic modelling of salinity and temperature (as well as velocity and sea-surface elevations) the model of James (1989) has been developed to include tides and wind-driven flow (density forcing and advection of density being included already). For simulation of the NSP period, boundary and initial conditions are taken from the 15-month 3D run described above whilst heat input is calculated from meteorological data following Lane (1989). The model successfully predicts the onset of the thermocline in spring, showing the frontal boundary between northern stratification and southern well-mixed waters. Initial runs (figure 2, plate 1) took place on a subset of the 15-month simulation grid, but more recently a 2.5 km version has been developed.

Suspended sediment transports can be simulated using the advection–diffusion equation. However, prescription of the sink (settlement) and source (erosion) terms has particular difficulties. Moreover, the settling velocities of coarse sand and fine clay particles differ by orders of magnitude; separate simulations for differing particle sizes are required. In deeper water with smaller tidal currents, vertical variability in the concentrations of all but the finest suspended sediment requires a full 3D representation.

Despite these difficulties, NSP observations of suspended sediments have yielded data within which specific components can be easily identified, namely (i) tidal current speed; (ii) semi-diurnal; (iii) spring-neap tidal; (iv) storm-surge currents; (v) wave; (vi) seasonal. Prandle *et al.* (this symposium) show how the spring-neap tidal component can vary according to both the (scaled) settling velocity w_s and intensity of vertical mixing (i.e. according to w_s/D and E/D^2, where E is the eddy viscosity parameter and D is the depth); the transport of sediments with $w_s < 10^{-6}$ m s^{-1} is shown to approximate that of a dissolved tracer. Jago *et al.* (this symposium) have shown how (i) and (ii) can be related via the dispersion equation to a combination of resuspension and advection along horizontal gradients of concentration. Furthermore, a 'point' turbulence energy model (Simpson & Sharples (1992), simulating velocity and density profiles) has been modified to include sediment resuspension and vertical mixing. Using two sediment populations and adjustable erosion, measured suspended sediment concentration profiles have been successfully simulated at a well-mixed site and during thermocline development (Jago *et al.*). Application of the two-layer model of Larsen *et al.* (1991) has given successful predictions of time-averaged bed shear stress in a wave/current flow for rough turbulent boundary conditions (Green *et al.* 1990; Jago *et al.*). However, changes in bed geometry and roughness hamper modelling of the enhanced resuspension processes under very energetic waves (Jago *et al.*).

3. Nutrients, oxygen and microbiology

The modelling of nutrient distributions is a useful starting point for studies of dispersed terrestrial inputs. Principal inputs to the North Sea are well known and are dominated by regularly monitored rivers. Nutrient measurement techniques are well established; measurements were made on all NSP survey cruises. This large nutrients data set makes a suitable test of models. Moreover, the significance of different processes changes through an annual cycle of concentration, corresponding to the biological growth and decay cycle. In late autumn and winter, biological processes can be neglected and a direct comparison made between monthly observed and modelled changes.

A particle-tracking model has been developed, incorporating random-walk diffusion; it follows the dispersion of a dissolved chemical species in meteorologically induced and tidal flows (from the 2D calculation above). A comparison with observed distributions (Howarth *et al.*, this symposium) suggests that most of the winter increase is due to regeneration; dissolved nitrate from suspended biological detritus and silicon from bottom sediments. The riverine inputs dominate only in a narrow coastal strip.

Mass balances of nutrients were found for three short cruises covering the Humber plume, using measurements for the nutrient field and a model for flow across the plume boundaries (figure 1). A time-evolving box model of nitrate, phosphate and silicate in the plume was also developed. Survey nutrient data upstream and downstream of the plume were used in inflow and outflow functions. A chlorophyll cycle based on monthly survey data gave stoichiometric nutrient uptakes. Comparison with total contents (from monthly surveys) and mass balances gave a check on the functions used. The results over the 15-month survey period show the changing balance between daily-gauged river supply, advective in/outflow, regeneration and uptake (figure 3).

A small net import by advection was found only during the local bloom, which consumed 80–170% of the annual river supply. Nutrient supply by advection during the winter and spring exceeds that due to the river. To support the spring bloom, an 'extra' source of nitrate (but not phosphate or silicate) is inferred, about twice the estimated nitrate and ammonia in rainfall. A chlorophyll growth model was incorporated in an advection–diffusion model of the Humber plume, to estimate spatial and temporal variations in primary production and hence nitrate sources, transport and usage. This approach enables construction of a plume budget for nitrate; application to other nutrients needs a better description of nutrient processes and phytoplankton speciation.

An alternative approach with more vertical structure is adopted in the 'point' model 'L3VMP' (Tett 1990). This describes simplified microbiology (photosynthesis and mineralization) in mixed layers above and below the thermocline (whose biology is incorporated in the upper layer) and in the oxic bioturbated layer of the sediment. Horizontal transports are neglected; local heating and stirring determine the stratification. There is air–sea gas-exchange. Tide- and wave-induced bed stress resuspends sediment, which absorbs light otherwise available for photosynthesis. The biological model combines phytoplankton and associated bacteria and protozoa in a microplankton compartment (variables C, N) with growth predicted by a cell-quota threshold-limitation model (Tett & Droop 1988). A detrital compartment (variables C, N) accounts for mineralization in the water column and sea bed. Differential equations for rates of change in each layer describe the production and consumption of oxygen and organic carbon, and the cycling of nitrogen through ammonium, nitrate and particulate organic matter. Predicted concentrations (Tett *et al.*, this symposium) agree well with NSP measurements of nitrate and chlorophyll (to a lesser degree). Continuous moored-fluorometer time series (Mills & Tett 1990) prove important for testing the modelled bloom. L3VMP has been useful in relating nutrients and plankton data to biological process experiments and to physical-oceanographic studies of stratification and sediment resuspension (Tett *et al.*)

NSP measurements have provided a rare seasonal time sequence of changes in dissolved *oxygen* distribution throughout the waters of a semi-enclosed shelf sea. Two important features were: marked super-saturation in Dutch and Belgian coastal waters during *Phaeocystis* algal blooms (spring 1989) and following thermal stratification in the northern North Sea; extensive areas of hypoxic water built up below the thermocline during late summer and autumn of both 1988 and 1989 (Purdie *et al.* 1993; Howarth *et al.*, this symposium).

To model such seasonal changes in dissolved oxygen distribution, the 1D microbiological model L3VMP has been incorporated into the general-purpose 2D advection-diffusion model of §5. The seven microbiological variables (microplankton

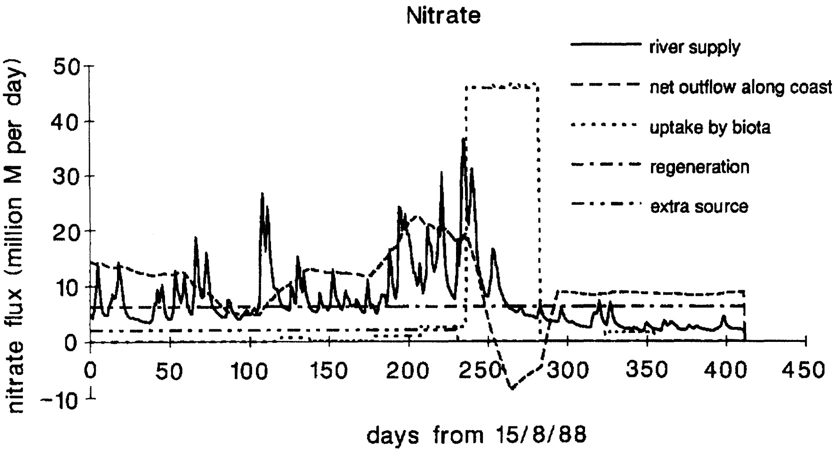

Figure 3. Nitrate balance from a time-evolving box model of the Humber plume. Trends for phosphate and silicate are similar, except that no 'extra' source is required for mass balance and the river supply is smaller, relative to regeneration and consumption during the bloom, than is the case for nitrate.

and detrital carbon and nitrogen; dissolved oxygen, ammonium and nitrate concentration) change (i) through advection and (ii) by the processes in the biological model. The combination has been used to predict the vertically integrated value of all seven variables in each 35 km grid cell covering the NSP survey area. To simplify combining the two models, the river input code was suppressed. As the hydrodynamic model is only 2D, a well-mixed or depth-averaged water column has been assumed. This is true all year in the southern North Sea, but clearly untrue in the summer-stratified waters of the northeastern and central parts of the North Sea.

Despite these model deficiencies, modelled oxygen distributions during spring approximate those from measurements in 1989 (figure 4, plate 2). Increased concentrations, caused by high rates of net phytoplankton productivity along the Belgian and Dutch coasts, are represented by the model. Later in the year, the model does not agree so well; depth-averaging of the data conceals the low sub-thermocline values. A two-layer model is expected to improve the model-data fit during the later summer months.

4. Metals

The NSP data now form one of the most comprehensive data-sets on dissolved and particulate trace metals for coastal waters. Seasonal and spatial variability are evident, allowing validation of broad-scale models. Moreover, the unusually extensive physical, biological and sedimentological data aids model development and interpretation. Sediment resuspension studies (Jago *et al.*, this symposium) emphasized the dependence of biogeochemical fluxes across the sediment/water interface on the nature and movement of near-bed particulate material. The bloom process cruise (Burton *et al.*, this symposium) allowed more detailed study of the interaction between metals and biota.

Much finer temporal and spatial resolution exists in the plume studies, and dissolved metal data from three Humber-plume cruises were used to calculate mass balances. Estuarine inputs were estimated from anchor station observations and a hydrodynamic model. Similarly, the observed metal field in the plume was interpolated and combined with residual flows from the hydrodynamic model to give fluxes within the plume. Hence estimates can be made of the balance between river input, consumption and cross-box flow, for the measured suite of metals: Fe, Mn, Cd, Al, Co, Cu, Ni, Pb and Zn.

Partitioning is a key process in the cycling and fate of metals in coastal waters (see also Burton *et al.*). The distribution coefficient K_d (Balls 1988) describes partitioning between particles (> 0.4 μm diameter) and dissolved metals (< 0.4 μm):

$$K_d = C_P/C_D,$$

where C_P is the metal concentration in particulates (mg per kg of particulate), C_D is the dissolved concentration (mg l^{-1}).

The processes operating at particle surfaces and leading to metal uptake are complex and range from active biological uptake by enzyme systems to simple cation adsorption and desorption (Morel *et al.* 1991). The K_d value thus subsumes a range of environmental mechanisms and varies with context; however, trends of values for specific elements are clear. Table 1 shows distribution coefficients determined during the NSP using radiotracers added to waters *in situ*, as well as from measured concentrations of corresponding stable isotopes. Radiochemical K_d values varied greatly, and depended on particle type. Relatively low values of K_d were obtained in estuarine plumes during winter when particles were primarily fluvial or resuspended. In contrast, K_d values for ^{109}Cd and ^{65}Zn are greatly enhanced for diatoms. *Phaeocystis* show a reduced particle affinity, particularly for ^{54}Mn, albeit higher than plume K_d values for ^{109}Cd and ^{65}Zn. These trends corroborate inferences made from stable ambient values of K_d (Turner *et al.* 1992). Hence particle composition strongly affects trace-element distributions and must be incorporated into models predicting trace-metal dispersion.

The clear trends also show that K_d provides a useful parametrization, particularly for the North Sea where field data can provide values appropriate to the context and season. However, dissolved-particulate transfer times may vary from hours to months (see Turner *et al.* (1992) and references therein). If the transfer is slow relative to the modelling time-step, then it appears as a source or sink term in the respective advection–diffusion equations. Rapid dissolved-particulate interactions correspond to thermodynamic equilibrium, for which trace-metal adsorption models can provide distribution coefficients (e.g. by the HALTAFALL computer code; Turner *et al.* 1991).

For metals in the Humber plume, a lack of such information limits the use of advection–diffusion models to calculate the metals' distribution. Nevertheless, the use of trace-metal adsorption models shows some promise for zinc, using also calculated conservative metal plumes and measured suspended sediment and temperature. Thus an export of dissolved zinc from the plume area (figure 1) was found in December, net consumption in May and a rough balance in August. The supply was dominated by advection from the north, exceeding estuarine inputs by factors 10–50 with increases during spring and summer.

To address the role of biological uptake, a 2D phytoplankton growth model of the plume has been developed to estimate daily primary production. Fixed carbon–metal ratios are assumed (equivalent to choosing K_d if uptake is moderate; when little dissolved metal remains, a change of carbon–metal ratio must occur). Metal removal during the bloom was thus estimated to be significant.

For a more detailed study of the biological cycle of *arsenic* (with chemistry analogous to phosphate) a plankton growth model was developed, without water-transport effects, for a depth-averaged box located in the Silver Pit area (53.6° N,

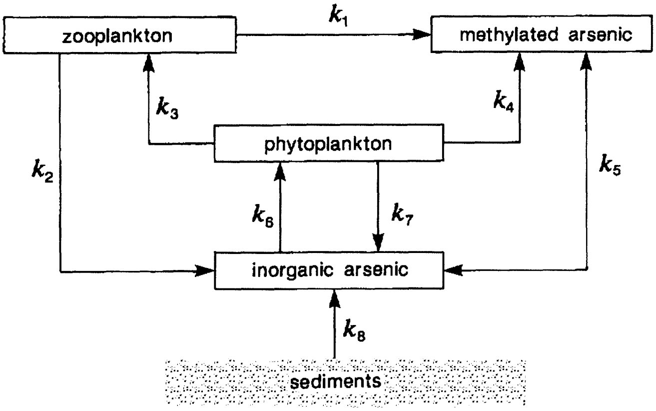

Figure 5. Arsenic cycling model in a 1 m^2 column of water, 60 m deep, located at Silver Pit in the North Sea (53.6° N, 0.9° E). The zero-order rate constants given below were based on NSP field measurements and literature data:

k_1	k_2	k_3	k_4	k_5	k_6	k_7	k_8
2.19	1.97	5.75	9.8	9.8	40	9.8 (all $\mu g\ m^{-3}\ d^{-1}$)	1 $\mu g\ m^{-2}\ d^{-1}$

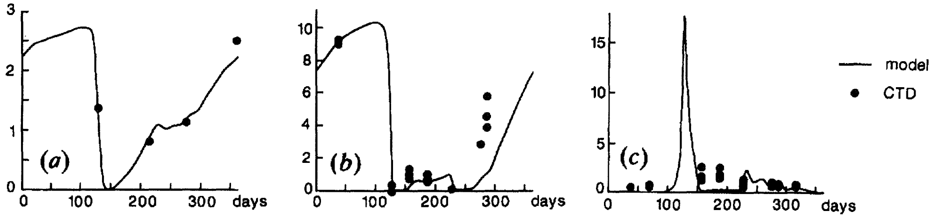

Figure 6. Predicted annual variation in (*a*) dissolved inorganic arsenic ($\mu g\ l^{-1}$); (*b*) nitrate ($\mu M\ l^{-1}$); (*c*) chlorophyll ($\mu g\ l^{-1}$), from the model in figure 5.

Table 1. *Distribution coefficients from* in situ *radio tracer experiments*

metal	Humber plume	Thames plume	diatom bloom	*Phaeocystis* bloom
^{109}Cd	400	530	7400	2100
^{137}Cs	510	310	ND[a]	ND[a]
^{54}Mn	53000	32000	86500	3900
^{65}Zn	5400	3700	29300	8100

[a] ND: plankton counts for ^{137}Cs were below the limit of detection.

0.9° E). Light, limiting nitrate and grazing by herbivores control bloom development (figure 5). Planktonic uptake k_6 (not previously determined in the North Sea) was obtained by incubating a large-volume water sample, containing 2 $\mu g\ l^{-1}$ of a growing plankton bloom, under constant conditions for six days. Measurements near the mouth of the Humber found arsenic effluxes k_8 from the sediments of 1 μg As $m^{-2}\ d^{-1}$ (negligible during the bloom, but possibly significant later). The predicted annual cycle (incorporating the measured rates k_6, k_8; figure 6) shows arsenic uptake only during plankton growth; the spring bloom consumed 80% of the winter maximum. The metal concentration then recovers slowly before a smaller, second depletion associated with the autumn bloom. Plankton growth soon ceases; dissolved arsenic reaches its winter maximum value after about 100 days. Figure 6 shows a good fit to the observations.

Measured and modelled concentrations of dissolved metals are compared in Prandle *et al.* (this symposium) on a time- and space-averaged basis. For spatial distributions, integration of geochemical processes with the general-purpose 2D model of §5 is underway, initially focusing on more conservative elements, e.g. Cu, Cd. Rivers have been taken as the principal initial input; *additions* for each grid unit use NSP data (atmospheric and benthic inputs) and others', e.g. the German ZISCH programme (Moll & Radach 1990); *removal* from solution and *cycling* use K_d concepts. (Boundary inputs from the Channel use data from FluxManche (Statham *et al.* 1993) and earlier estimates. The northern boundary conditions are poorly defined; present data suggest a small net off-shelf export of some metals (Hydes & Kremling 1993); the most reliable available estimates from the NSP survey grid are used.) The model results of these processes and dispersion are tested by measured NSP distributions; divergences indicate missing or poorly modelled processes.

5. Strategy and framework

The preceding account illustrates the many specialisms to be combined in any sophisticated water quality model. A 'framework' is needed to facilitate parallel advances by specialists and then harness the different components.

As many as 100 scientists from 20 separate organisations participated in the NSP, emphasizing the scope for parallel model development. The basis is common hydrodynamics and advection–diffusion physics (§§1, 2). To encourage widespread use, a simple but not idealized model was formulated, namely 2D hydrodynamics for simulating tidal and wind-driven currents (vertically-averaged) over periods of up to several years. This 'general-purpose' model incorporated an advection-diffusion module that also simulated localized sink and source terms. (In some applications, only this module was used, tidal and wind-driven currents being specified from separate model runs. Modules for data analysis and presentation were also incorporated.) A modular structure enabled users readily to include their specific algorithm, despite perhaps limited familiarity overall. A detailed user manual included continual updates for specific module developments.

The model was used by 20 scientists for applications directly linked to the NSP: simulation of currents and North Sea distributions of temperature, salinity, suspended sediments, nutrients, O_2, microbiology and metals. (Further uses have included fish larvae distributions, applications in the Humber, eastern Irish Sea and across the whole north-west European continental shelf, and copies for university teaching.) Necessary support for these model transfers varied: typically an initial day or so if the receiving group included an experienced mathematician or physicist; occasionally development of an appropriate version to simulate a specific tracer.

Substantial software development is required for the model robustness and clarity needed in such general application. Moreover, the initial support for model transfers far outweighed the effort that would have been required to run all simulations centrally. However, experienced modellers in the community resulted, so that a wide range of NSP observations was interpreted through modelling simulations (e.g. dissolved nutrient levels and oxygen saturation, §3). Benefits of integration within a modelling framework also became apparent, notably interaction between disciplines.

To harness a range of specialist components, the framework program of Wolf (1991) defines the interface (inputs and outputs in FORTRAN 'call' and 'common' statements) between the specialist aspect (expressed in a module updating the respective constituent variables) and the rest of the model. Moreover, specialist modules can be developed, and improved forms substituted, aiding their parallel development. Many interactions of the GESAMP (1991) conceptual model are incorporated; the program implements a flow chart with current, sediment, constituent and biological 'black-box' modules. Consistent with §1, many constituent modules call a common advection–diffusion module, which can thus receive special attention to its severe numerical challenge.

There is interaction between all processes in the model as the whole sequence of constituent updates is repeated, on an overall time-step chosen according to the processes which are to be resolved rather than parametrized. (A time-step of $\frac{1}{4}$ hour is widely appropriate, for tides, weather effects, sediment suspension, day–night heating and light, biological migration and plankton growth. Individual modules may have a shorter internal time-step, e.g. for numerical reasons.)

Such a common time-step, and common spatial structure, are strong constraints. Thus consistent space and time scales are more important than 'disciplinary' scope, when implementing the framework with different constituents (the insertion of additional constituent modules in parallel with those already present is relatively easy).

The framework has been successfully compiled with the simultaneous inclusion of modules for turbulence, suspended sediment and microbiology in 1D (vertical).

6. Outlook

There remains scope for further development of all aspects of water quality models.

Physical aspects include distinct shelf-edge and nearshore dynamics. The latter involve especially wave-induced mixing and possibly restratification by freshwater inflows (Simpson *et al.* 1993). Various contributions to dispersion remain to be quantified (cf. §2) and a model formulation is needed to advect sharp frontal and thermocline gradients without excess numerical diffusion or rippling. Regarding turbulent mixing, work is in progress to include stratification effects and there is a need for further research on the role of wind–waves and of internal waves (e.g. on the thermocline) and for careful testing of models against turbulence measurements.

There remains a need for improved representation of bed sediments: (i) erodibility according to cohesion and bioturbation; (ii) internal processes at different levels rather than a one-layer aggregate interacting only as a boundary condition (flux) for the bottom of the water column. Continuous measurements of vertical profiles (Jago *et al.*, this symposium) form a basis for developing suspended sediment models.

Modelling of sediments and especially biological variables may benefit from a particle-tracking approach allowing more explicit representation of particle history.

The study, numerical formulation and model-testing for all processes is preferably carried out in contexts where they can be isolated, to avoid complexity and aid rigorous testing and diagnosis of model-measurement discrepancies. (A certain level of accuracy might be more readily shown for a '0D' 'box' model, than for all aspects of a 3D model.) There is a need for explicit consideration of the balance between sophistication for detailed simulation and simplicity for development, testing and diagnosis.

Management and policy applications of water-quality models should allow time to exploit tested sophisticated models appropriate to the problem. By contrast, accidents may call for quick results, operational use, and convenience (e.g. reduced inputs and outputs) rather than sophistication.

A framework as in §5 allows some flexibility in substituting simpler or more sophisticated modules. General improvements or specialised modules targeted at specific problems may also be substituted in an evolutionary way.

How useful are such frameworks to scientific research as distinct from management? The example in §5 took just a few days to write, demonstrating flexibility in frameworks *per se*; the inhibiting effort is in adapting existing specialist routines as modules (i.e. to match with each other). Matching and its scientific benefits will be encouraged if the interface 'seen' by the specialist module is stable, independent of the particular problem (or even of water-quality interest). This suggests that the problem-dependent aggregation of modules, timescale, etc., be subsumed in flexible forms of framework.

Flexibility may be assisted by 'off-line' runs of any model components that are sequential rather than interactive. For example, a shelf-wide model may be run first if required only for tidal and wind-driven input to nearshore scenarios.

Computing power is a constraint. Modelling of 3D physics for a moderate area is possible on individual workstations, and a one-year run for the North Sea with $2\frac{1}{2}$ km resolution (barely resolving the internal radius of deformation) is just feasible on a present supercomputer. Finer resolution is possible locally. Nevertheless, reductions in grid size, and extensions of sea area and time duration, will fill the most powerful supercomputers foreseen. Other water-quality (and ecological) variables require (much) more computation at each point.

Large models require much input data and the means to handle, display and gain insight from the vast quantity of model output. Even bathymetry poses a continuing problem for models finer than the 2 km gridded set now being prepared (M. T. Jones, personal communication). Hourly values for 15 months from the $2\frac{1}{2}$ km resolution 3D model of southern North Sea physics amount to O(300 Gbytes). Given that local transports derive from shelf-wide forcing with relatively small computing demands, the issue becomes: how far across the shelf is it *convenient* to extend the resolution and level of sophistication required in the area of interest.

Trace metals exemplify limited (input) data availability. Methods are needed to measure their distributions with much improved spatial and temporal resolution, to improve understanding of their marine geochemistry, refine models and progress towards a predictive capability.

Coupled models are expected to make a large contribution to understanding the effects of changes in estuarine pollutant inputs into the North Sea, and to its strategic management (Klomp 1990). The North Sea Task Force is attempting to rationalize the modelling of pollutant transports (Hoogweg *et al.* 1991).

Immediate plans following the work described herein are to simulate August 1988 to October 1989 with the 3D $2\frac{1}{2}$ km prognostic physics model, and to make these data readily accessible to the scientific community. Modelling of other constituents continues to develop as described above. It is planned to implement the framework (i) in nearshore contexts (interactions of wind and wave stirring, fresh-water stratification, sediment resuspension, light, nutrients and primary production), (ii) off northeast England as part of the Land–Ocean Interaction Study (LOIS), (iii) extending the area of $2\frac{1}{2}$ km resolution and also embracing fine resolution over the Hebrides Shelf edge. Discrete releases of technetium from Sellafield in 1993, and the expected subsequent transport around Scotland into the North Sea, provide the prospect of a unique data set to test such a model's ability to simulate shelf-wide transports and ocean-shelf exchange.

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References

Backhaus, J. O. & Hainbucher, D. 1987 A finite difference general circulation model for shelf seas and its application to low frequency variability on the north European shelf. In *Three-dimensional models of marine and estuarine dynamics* (ed. J. C. J. Nihoul & B. M. Jamart). Elsevier Oceanography Series, vol. 45, pp. 221–224.

Balls, P. W. 1988 The control of trace metal concentrations in coastal seawater through partition onto suspended particulate matter. *Neth. J. Sea Res.* **22**, 213–218.

Bewers, J. M., *et al.* 1992 A conceptual model of contaminant transport in coastal marine systems. *Ambio* **21**, 166–169.

Billen, G., Lancelot, C., DeBecker, E. & Servais, P. 1988 Modelling microbial processes (phyto and bacterioplankton) in the Schelde estuary. *Hydrol. Bull.* **22**, 43–55.

Davies, A. G. 1990 A model of the vertical structure of the wave and current bottom boundary layer. In *Modeling marine systems* (ed. A. M. Davies), vol. 2, pp. 263–297. Boca Raton, Florida: CRC Press.

Davies, A. M. & Jones, J. E. 1991 Application of a three dimensional turbulence energy model to the determination of tidal currents on the Northwest European Continental Shelf. *J. geophys. Res.* **95**, 18,143–18,162.

Durazo-Arvizu, R., Hill, A. E., Smeed, D. A. & Linden, P. F. 1993 Horizontal circulation at a tidal mixing front in the North Sea. *Continental Shelf Res.* (In the press.)

Elliott, A. J. 1986 Shear diffusion and the spread of oil in the surface layers of the North Sea. *Dt. hydrogr. Z.* **39**, 113–137.

Fransz, H. G., Mommaerts, J. P. & Radach, G. 1991 Ecological Modelling of the North Sea. *Neth. J. Sea Res.* **28**, 67–140.

GESAMP (IMO/FAO/UNESCO/WMO/WHO/IAEA/UN/UNEP joint Group of Experts on the Scientific Aspects of Marine Pollution) 1991 Coastal Modelling. *GESAMP Rep. Studies, IAEA* **43**, 191 pp.

Grant, W. D. & Madsen, O. S. 1986 The continental-shelf bottom boundary layer. *A. Rev. Fluid Mech.* **18**, 265–305.

Green, M. O., Rees, J. A. & Pearson, N. D. 1990 Evidence for the influence of wave-current interaction in a tidal boundary layer. *J. geophys. Res.* **95**, 9629–9644.

Hoogweg, P., DuCrotoy, J.-P. & van der Wetering, B. 1991 The North Sea Task Force: the first two years. *Mar. Poll. Bull.* **22**, 328–330.

Huthnance, J. M. 1988 Oceanographic modelling. *Underwater Technol.* **14**, 3–8.

Huthnance, J. M. 1991 Physical oceanography of the North Sea. *Ocean Shoreline Management* **16**, 199–231.

Hydes, D. J. & Kremling, K. 1993 Patchiness in dissolved metals (Al, Cd, Co, Cu, Mn, Ni) in North Sea surface waters: seasonal differences and influence of suspended sediment. *Cont. Shelf Res.* (In the press.)

James, I. D. 1989 A three-dimensional model of circulation in a frontal region of the North Sea. *Dt. hydrogr. Z.* **42**, 231–247.

Klomp, R. 1990 Modelling the transport and fate of toxics in the southern North Sea. *Sci. Total Env.* **97**, 103–114.

Lane, A. 1989 The heat balance of the North Sea. *Proudman Oceanogr. Lab. Rep.* **8**, 46 pp.

Larsen, L. H., Sternbery, R. W., Shi, N. C., Marsden, M. A. H. & Thomas, L. 1981 Field observations of the threshold of grain motion by ocean waves and currents. *Mar. Geol.* **42**, 105–132.

Moll, A. & Radach, G. (eds) 1990 ZISCH parameter report: compilation of measurements from two interdisciplinary STAR-shaped surveys in the North Sea. *Institut für Meereskunde, Hamburg, Tech. Rep.* 4–90, 7–90.

Mills, D. K. & Tett, P. B. 1990 Use of a recording fluorometer for continuous measurement of phytoplankton concentration. *SPIE Proc.* **1269**, 106–115.

Morel, F. M. M., Dzombak, D. A. & Price, N. M. 1991 Heterogeneous reactions in coastal waters. In *Ocean margin processes in global change* (ed. R. F. C. Mantoura, J.-M. Martin & R. Wollast), pp. 165–180. Chichester: Wiley.

Prandle, D. 1984 A modelling study of the mixing of ^{137}Cs in the seas of the European continental shelf. *Phil. Trans. R. Soc. Lond.* A **310**, 407–436.

Proctor, R. & Smith, J. 1991 The depth-averaged residual circulation on the North West European Shelf. *Proudman Oceanogr. Lab. Rep.* **20**, 255 pp.

Purdie, D. A., Daneri, G., Plummer, D. H. & Thomson, S. 1993 The seasonal distribution of dissolved oxygen in the southern North Sea. (In preparation.)

Riepma, H. W. 1985 Current meter records and the problem of the simulation of particle motions in the North Sea near the Dutch coast. *Oceanol. Acta* **8**, 403–412.

Røed, L.-P. & Cooper, C. K. 1986 Open boundary conditions in numerical ocean models. In *Advanced physical oceanographic numerical modelling* (ed. J. J. O'Brien), *NATO ASI* C **186**, 411–436. Dordrecht: Reidel.

Simpson, J. H. & Sharples, J. 1992 Dynamically active models in the prediction of estuarine stratification. In *Dynamics and exchanges in estuaries and the coastal zone* (ed. D. Prandle), pp. 101–113. New York: Springer-Verlag.

Simpson, J. H., *et al.* 1993 Periodic stratification in the Rhine ROFI in the North Sea. *Oceanol. Acta.* **16**, 23–31.

Stigebrandt, A. & Wulff, F. 1987 A model of dynamics of nutrients and oxygen in the Baltic proper. *J. mar. Res.* **45**, 729–759.

Statham, P. J., *et al.* 1993 Fluxes of Cd, Co, Cu, Fe, Mn, Ni, Pb and Zn through the Strait of Dover into the Southern North Sea. *Oceanol. Acta.* (Submitted.)

Tett, P. 1990 A three layer vertical and mirobiological processes model for shelf seas. *Proudman Oceanogr. Lab. Rep.* **14**, 85 pp.

Tett, P. & Droop, M. R. 1988 Cell quota models and planktonic primary production. In *Handbook of laboratory model systems for microbial ecosystems* (ed. J. W. T. Wimpenny), vol. 2, pp. 177–233. Florida: CRC Press.

Turner, A., Millward, G. E., Bale, A. J. & Morris, A. W. 1992 The solid–solution partitioning of trace metals in the southern North Sea – *in situ* radio chemical experiments. *Cont. Shelf Res.* **12**, 1311–1329.

Turner, D. R., *et al.* 1991 Surface complexation modelling of plutonium adsorption on sediments in the Esk estuary, Cumbria. In *Radionuclides in the study of marine processes* (ed. P. J. Kershaw & D. S. Woodhead), pp. 165–174. London: Elsevier.

van Eck, G. Th M. & de Rooij, N. M. 1990 Development of a water quality and bio-accumulation model for the Scheldt Estuary. In *Estuarine water quality management* (ed. W. Michaelis). *Estuarine coast. Stud.* **36**, 95–104. Berlin: Springer-Verlag.

Wolf, J. 1991 A unified framework for water quality modelling shallow seas. *Proudman Oceanogr. Lab. Rep.* **19**, 46 pp.

Zimmerman, J. T. F. 1986 The tidal whirlpool: a review of horizontal dispersion by tidal and residual currents. *Neth. J. Sea Res.* **20**, 133–154.

Discussion

P. J. Radford (*Plymouth Marine Laboratory, U.K.*). It is perhaps not surprising that physicists should conceive that an ecosystem should be represented as a simple ‘source or sink’ term in an otherwise sophisticated hydrodynamic advective–dispersive partial differential equation. Ecologists have also tended to represent ecosystems as a complex interaction of biological processes such as primary production, feeding, respiration, defecation, predation and exudation modified by a simple 'transport' term. Interdisciplinary research encourages a more holistic understanding of ecosystems where each module is given equal importance and is equally prone to modification and replacement as research dictates. The European Regional Seas Ecosystem Model (ERSEM) is a project partly funded by the CEC under MAST that has adopted this approach. The partners from the eight participating European countries produce modules, such as primary production, zooplankton, the small food web, benthos and physical processes, which are combined to produce the ecosystem mode. Such a model may seem very complicated, and it has been argued that we should start with simple models and add complexity as necessary. However, I believe that if we proceed in such a manner we will never achieve our ultimate object of a complete ecosystem model. In general stepwise development has not taken many steps and yet the one or two holistic approaches have yielded useful models. The ERSEM formulation is considered by its creators to be the simplest model which can adequately describe the whole ecosystem including the recycling of nutrients and carbon with the realistic cycling times implied by the various temporary storage variables (dead organic carbon fractions and the microbial loop). Another important reason for including all of the ERSEM state variables is that they are of intrinsic interest to the ecologist. Phytoplankton may only be considered as a non-conservative state variable to a physicist but it is life sustaining food to a zooplankton population. We must also study the ecosystem as the environment from which we obtain our own food supplies, and try to predict the impact of anthropogenic change on fisheries. The whole ERSEM program is engineered with SESAME (Software Environment for the Simulation and Analysis of Marine Ecosystems). Within ERSEM the hydrodynamic regime may be replaced by a new module as simply as any of the other modules. The ecological model considers some 50 state variables including four nutrients, 14 living and eight non-living components in both the pelagic and benthic systems. In ERSEM I it has been applied simultaneously to the 10 surface ICES boxes of the North Sea plus the five ICES boxes below 30 m depth. The water transports are represented by data summaries obtained from a detailed (21 × 23 km) advective–dispersive model developed by Backhaus (1990). In the next phase of the ERSEM program (MAST II–ERSEM II) the same ecological model will be applied to the coastal strip of Eastern England in region of the Humber Plume. The Backhaus model will be used to define transports on a much finer geographical grid than that used in ERSEM I, needing 100–200 compartments.

Additional reference

Backhaus, J. O. 1990 On the atmospherically induced variability of the circulation of the Northwest European Shelf Sea and related phenomena – a model experiment. In *Modelling marine systems* (ed. A. M. Davies), vol. I, pp. 93–134.

J. M. HUTHNANCE. Philip Radford shows physical transports as a component of the ERSEM model, and the framework of Wolf (1991) shows the inclusion of biological processes and variables in a physical-transport framework. This complementarity shows that the issue is not the combination of physical, biological and other variables *per se*. A rather different and more difficult issue is illustrated by the coarse resolution of ERSEM I relative to almost all physical process models; agreement is needed on the spatial and temporal resolution required for the model to represent the physical and biological processes considered to be important.

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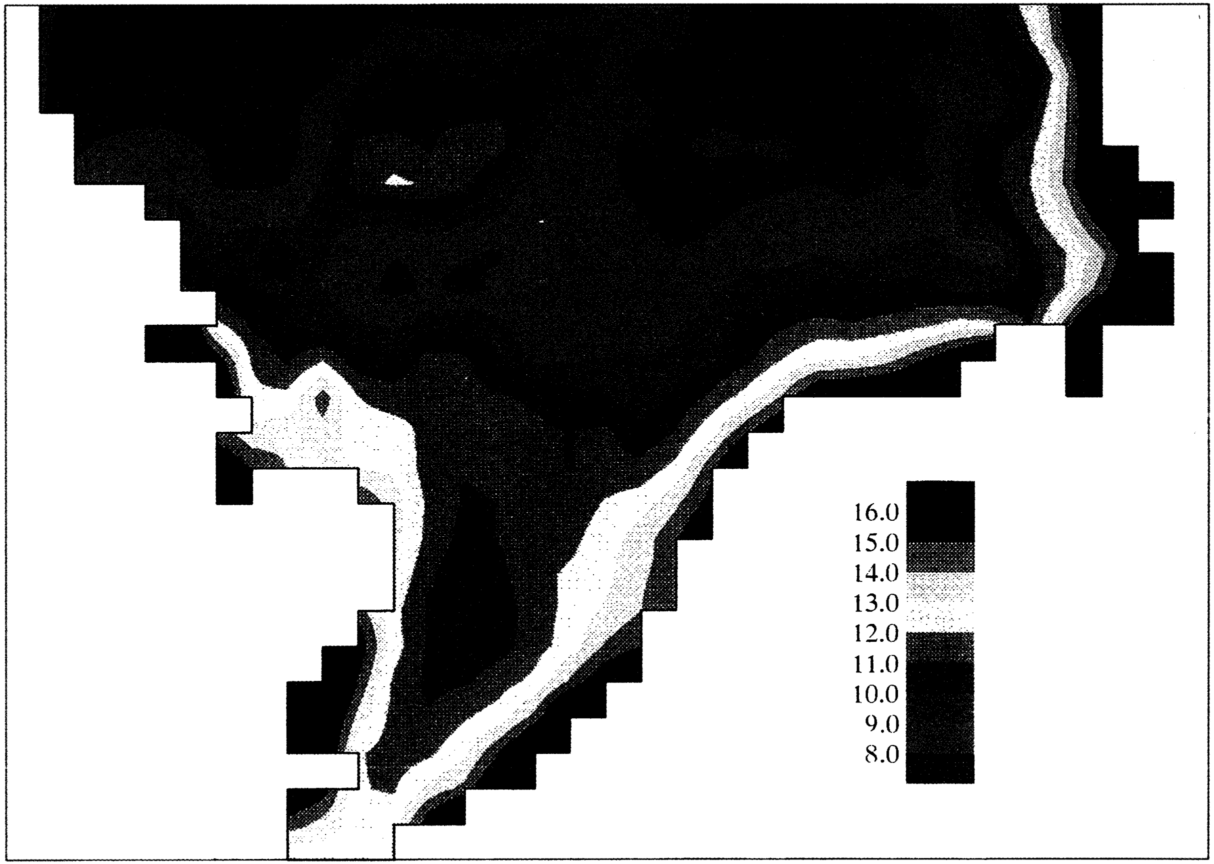


Figure 2. Sea-bed temperature, 2 June 1989, after two months integration of three-dimensional prognostic model from well-mixed conditions. The developed front can be seen extending from northeast England to the north Dutch and German coasts.

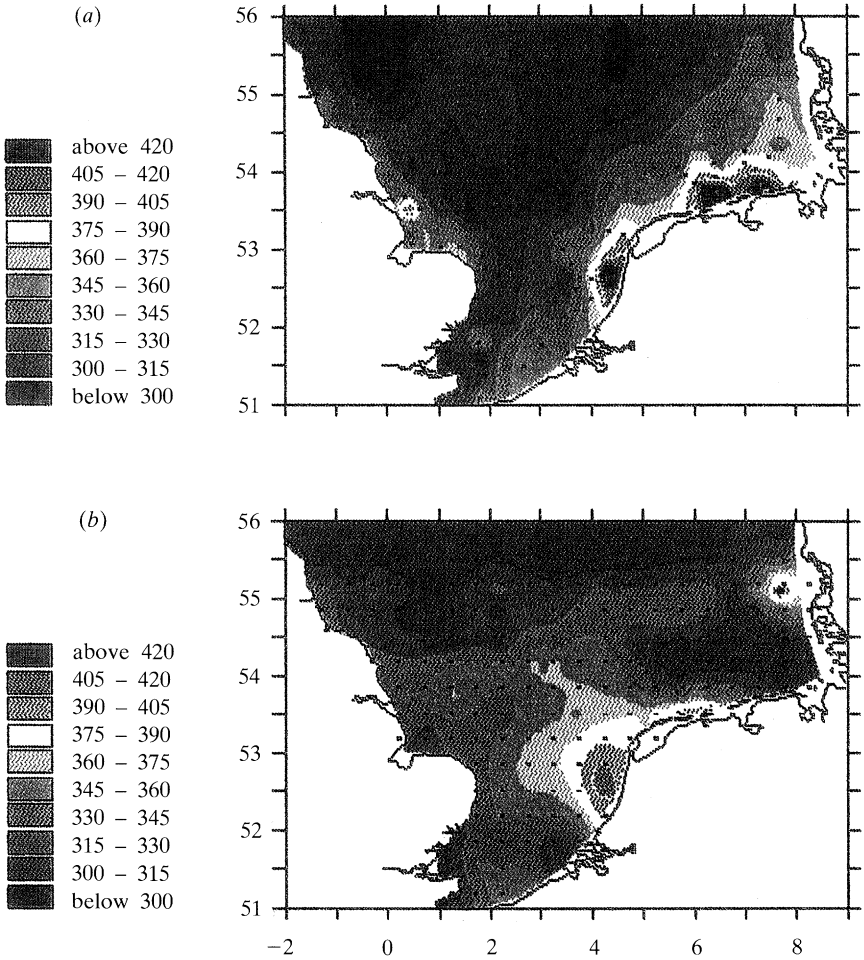
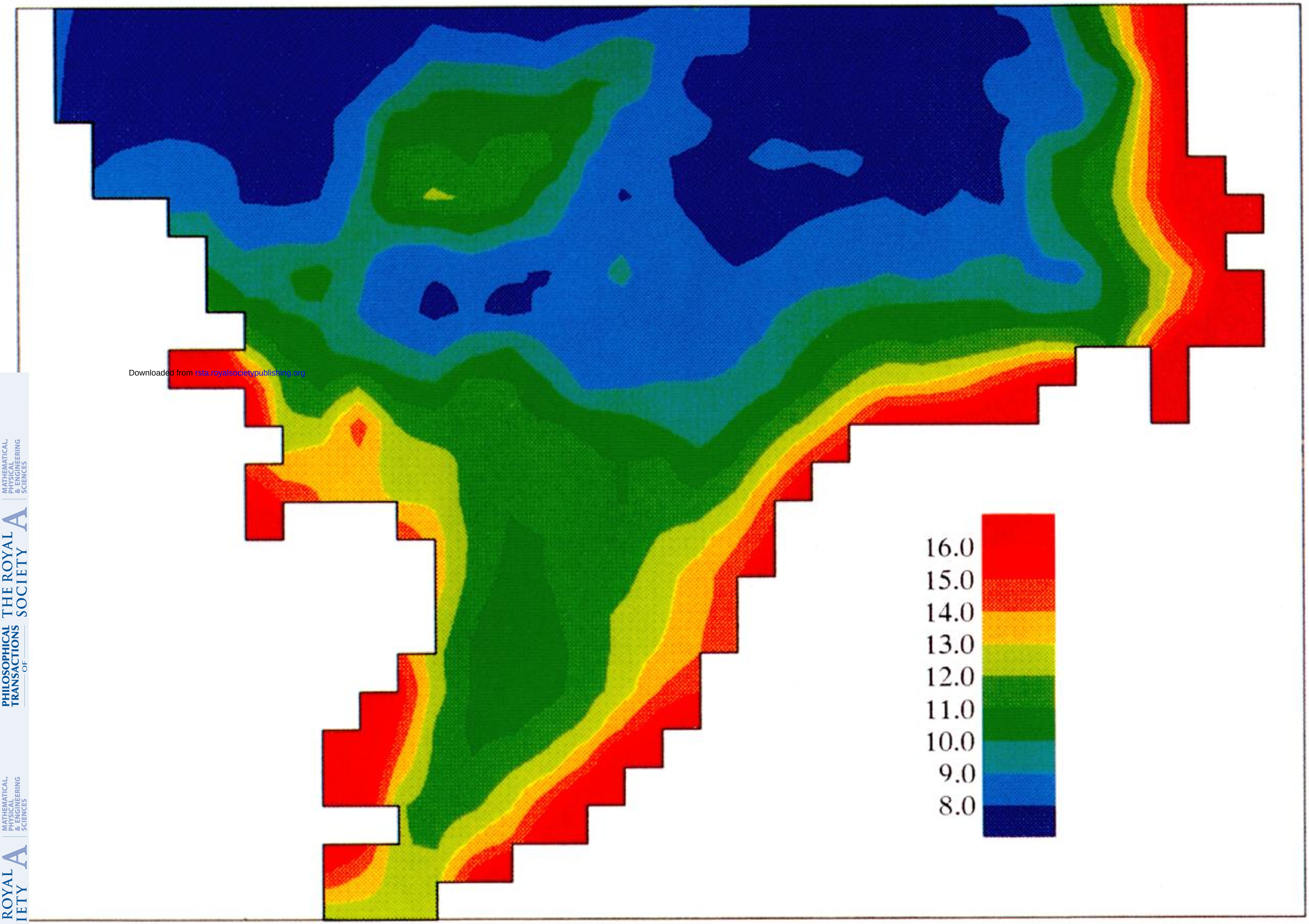


Figure 4. Observed surface dissolved oxygen concentration for April / May 1989 in the southern North Sea (*a*) and output for April 30 from a depth-averaged microbiological model incorporated into a two-dimensional hydrodynamical model of the same region (*b*). Units μM O_2 l^{-1}.



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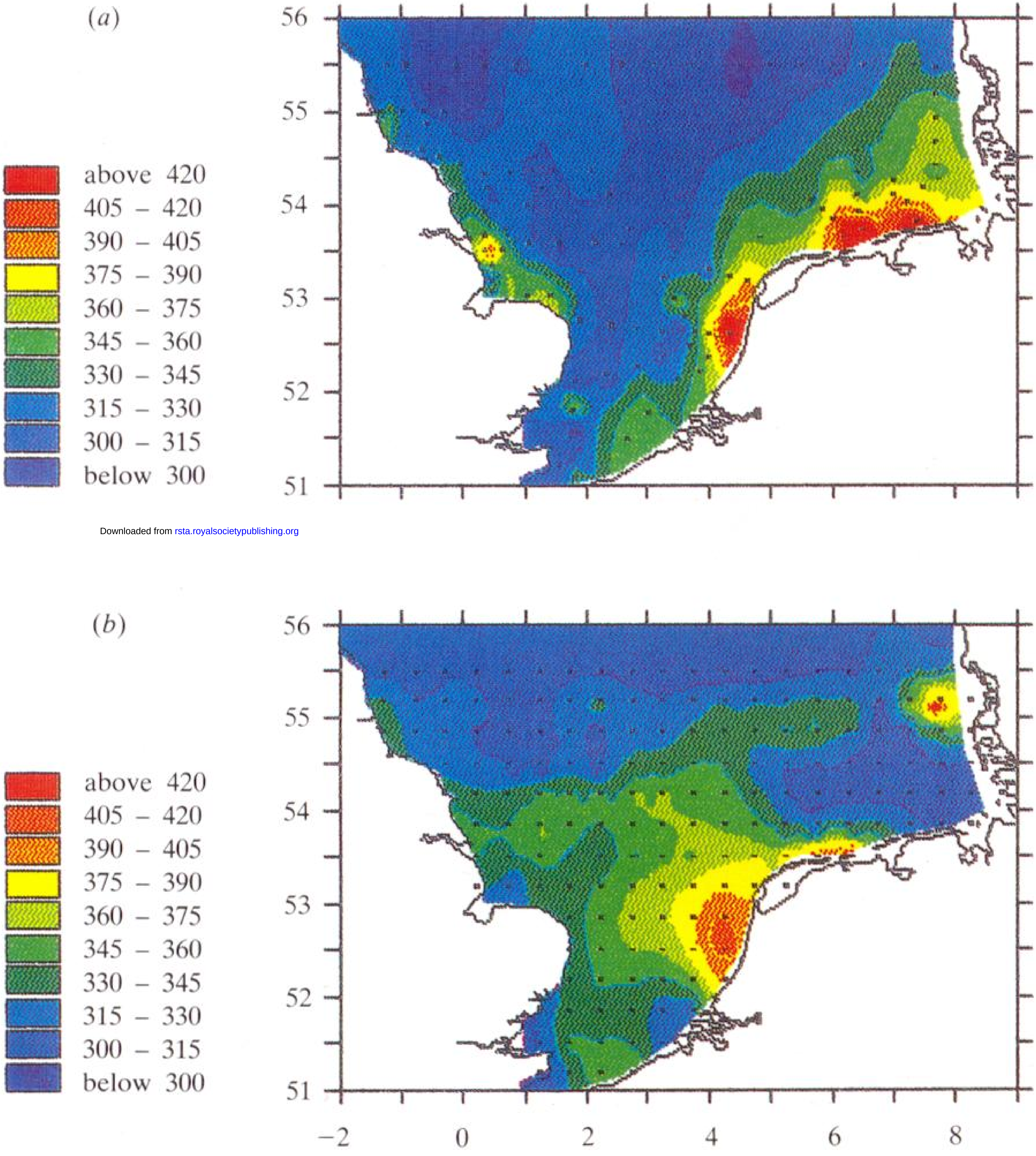

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