1992/060

RACS(R) CORE MODELLING PROJECT

by

P G Whitehead

Head of Environmental Hydrology
Institute of Hydrology
Wallingford

1. INTRODUCTION AND BACKGROUND

The LOIS project will investigate the complex physical, chemical and biological interactions occurring at the coastal zone. In addition the project will assess the impact of inputs from land surface, atmosphere, oceans and seas on coastal ecosystems. The time scales of interactions and impacts cover the last 200 years, the last two millennia and the Holocene period as a whole. LOIS will provide predictions of responses of coastal ecosystems to future changes on time scales of up to 200 years.

Given the complex, dynamic and multidisciplinary nature of the LOIS project it is inevitable that models will play a major role. Models allow an assessment of the processes controlling dynamic behaviour, can be operated at a number of different time scales and can be used to reconstruct historical behaviour patterns as well as providing predictive future scenarios.

As shown in Figure 1 there are many component parts of land-coast-sea and ocean systems that could be incorporated into LOIS. Many of these will be investigated during the LOIS programme. A major driving factor controlling estuary and coastal ecosystems is the inputs of water, sediments and chemical constituents derived from catchments, rivers and groundwater systems. These provide a constant stimulus to coastal systems and the measurement and modelling of fluxes is a cornerstone of the LOIS programme.

LOIS is centred on the East Coast rivers from the TWEED to the WASH (see Figure 2) and it is imperative that any modelling strategy provides consistent information on all of major river systems.

2. SPECIFIC OBJECTIVES

The specific objectives of the RACS are:

a) To measure, characterise and model the variability of contemporary fluxes of materials, including water, sediments, nutrients, organic matter and pollutants, into and out of the coastal zone.

b) To identify and quantify the chemical and biological transformation processes within river basins, the coastal zone and atmosphere that govern such fluxes.

c) To determine through observational and modelling studies how changes in land use, sea-level and other environmental conditions affect riverine and coastal ecosystems, with emphasis on the sustainability of living resources, on organic matter fluxes, and on geomorphological and geochemical processes in the coastal zone.

Modelling of catchments, rivers and groundwater is fundamental to RACS and this is emphasised in Appendix 1 which gives a summary of the RACS implementation plan. The modelling of inputs to the North Seas is reflected in the objectives of NORMS (see Appendix 2).

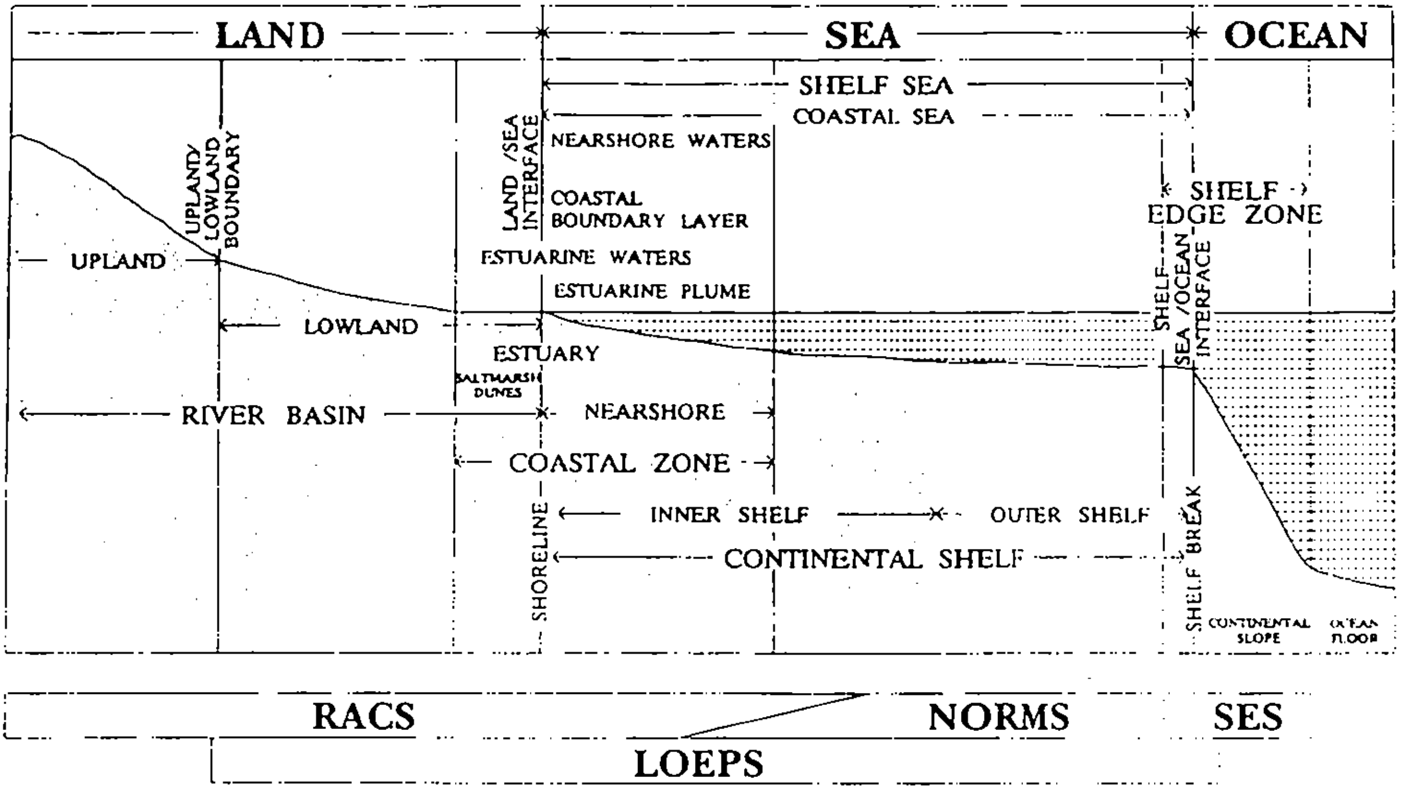


Figure 1 The application of names and terms used in the LOIS Science Plan in relation to the main studies. Those shown above the land surface – sea/ocean bed profile are of hydrological or oceanographic significance, while those below are physiographic (not to scale).

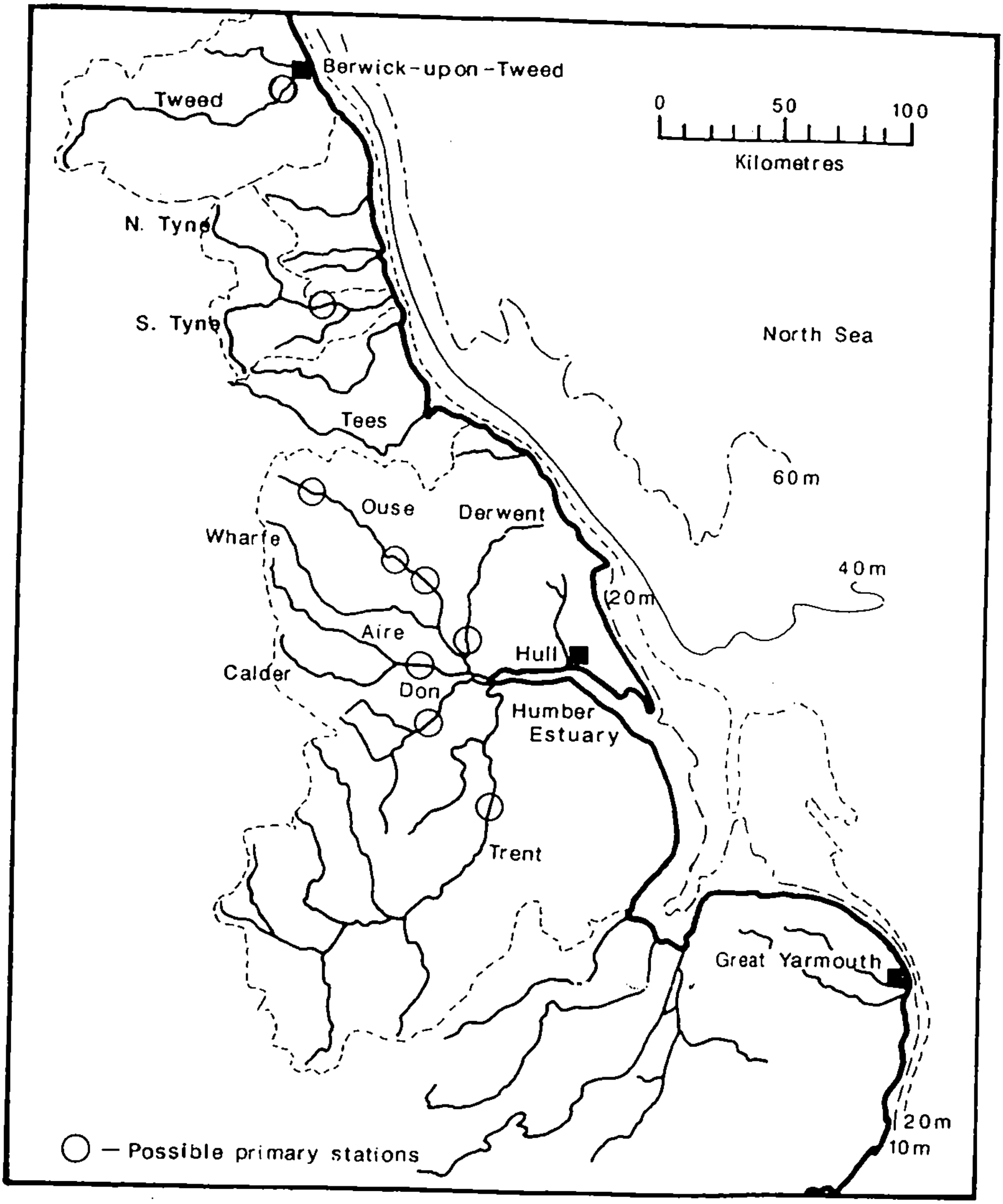


Figure 2 The RACS study site on the east coast of Britain showing the catchment systems and possible primary observation stations for the River Basin studies. Sampling for the Coast and Estuaries studies will focus initially on the coastal boundary layer between Berwick and Great Yarmouth extending up to 50 km offshore, and on the Humber Estuary and associated plume. One or more lines of stations extending offshore > 100 km are likely to be established in order to examine gradients in water and sediment properties away from land.

In terms of modelling the specific objectives are to:

a) identify and characterise the key processes controlling flow, sediment and chemical constituents in East Coast Rivers;

b) construct a range of mathematical models for the East Coast River Basins for flow, sediment and chemical constituents;

c) compute the contemporary land-to-sea fluxes of water sediment, biological matter, major dissolved constituents, nutrients and chemical contaminants;

d) reconstruct historical sequences of fluxes from changes in land use, past climates and other major perturbations within river basins;

e) predict the future fluxes given likely changes in land use and climate;

f) deliver to coastal and estuary modellers relevant data and simulations as inputs to estuarine and coastal models.

3. OVERALL MODELLING METHODOLOGY AND APPROACH

In order to meet the RACS(R) and LOIS objectives a number of component models need to be developed. There are shown in Figure 3 and consist of:

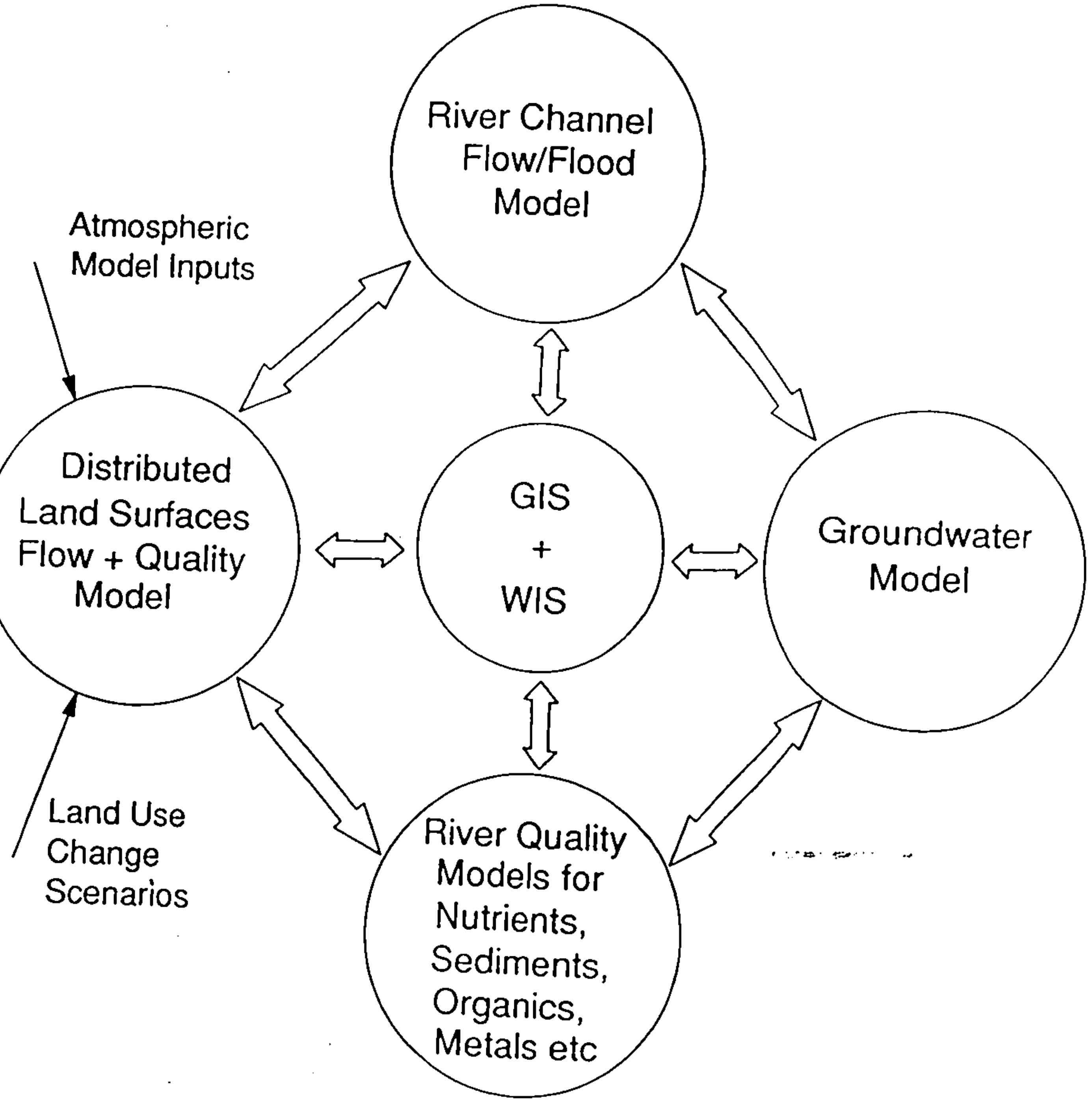
a) A distributed land surface flow and quality model. This will consist of 2D and 3D models which will translate rainfall into runoff using physically based hydrodynamic equations. Reduced order models will be developed for application on a 0.1 - 1km grid basis and will be expanded to include sediments, carbon, nitrates, metals and organics.

b) A river channel model will be developed for east coast rivers to compute flows and fluxes of constituents at key downstream locations. The model will operate at a range of time scales and will account for natural runoff from catchments sub-models and direct discharges of effluents into east coast rivers. Chemical and biological sub-models will be used for process interaction studies.

c) The movement of water and pollutants from aquifers to river and coastal systems will be a key feature of the RACS(R) core modelling programme. 2D and 3D models will be developed.

The overall modelling methodology will be strongly influenced by the objectives in section 2 of this report. As indicated in Figure 4 there are always alternative modelling approaches to any particular problem and these can range from solutions of complex non-linear differential equations through to relatively simple lumped models. At the same time data will be collected as part of the LOIS core chemistry projects and there will be a need for modellers to influence the data collection to ensure that model structure and detail is matched by data availability. The modelling process as illustrated in Figure 4 is to

LOIS CATCHMENTS/RIVER CORE
CORE MODELLING PROGRAMME



Databases Available - Land Use, HOST, Digital Terrain, Flow, Rainfall, Evaporation, Temperature, NRA Chemistry, River Network, Air Pollution Deposition Maps, etc.

Figure 3

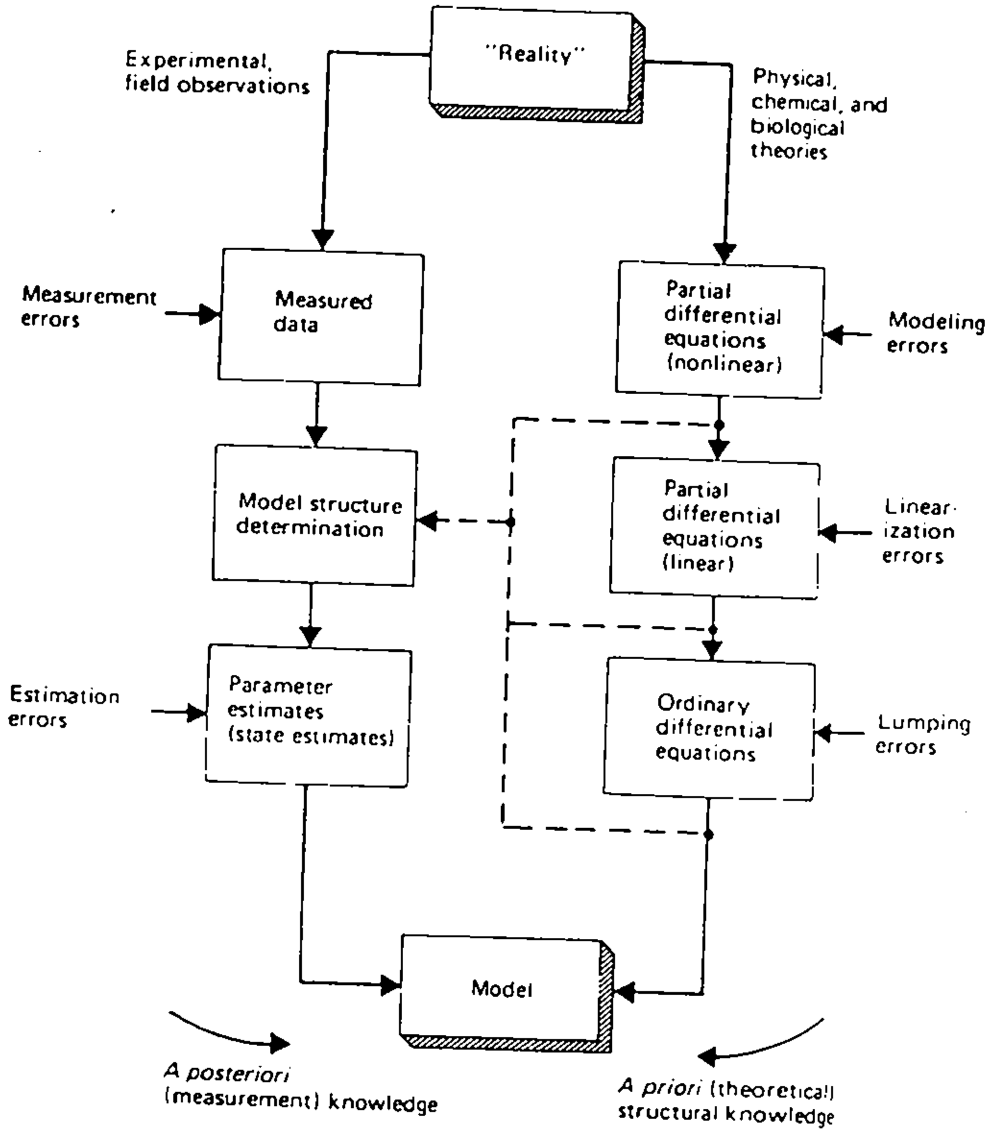


FIGURE 4 Combining *a priori* and *a posteriori* knowledge in the modeling procedure (adapted from Eykhoff, 1974).

combine the knowledge of structure and process with knowledge derived from measurements. In this way a consistent and compatible set of models will be developed which should meet the RACS and LOIS objectives.

4. COMPONENT SIMULATION MODELS

4.1 Catchment Flow

Land Surface Hydrology The catchment rainfall-runoff model for LOIS will draw on a long history of catchment modelling in the UK. Figure 5 shows the major features required in a generalised distributed model. These include

a) above ground models to represent the processes of canopy interception of rainfall and snow;

b) surface modules to describe snowmelt and evaporation processes;

c) root zone models for water uptake and soil water exchange processes;

d) soil zone models for water transfer vertically or laterally;

e) overland and channel flow model;

f) groundwater flow models.

Several catchment scale flow models have been developed. A number of models incorporating both surface and subsurface components have been developed by NERC. Such models are suitable for describing the movement of water through a catchment at a range of grid scales. They give a profile of soil moisture content and have dynamics determined by topography and soil properties, both specified at the same scale. Surface vegetation models and evaporation routines are included and they are coupled to channel flow routing components based on the kinematic wave approximation. These models can be viewed as a system of spatially linked saturated-unsaturated flow models taking topography into account.

The Institute of Hydrology Distributed Model (IHDM) incorporates spatial variability via a grid system. The grid is defined in plan by hillslope areas bounded by flowplanes which are assumed vertical and invariant (Figure 6a). Representative vertical planes are modelled by finite element approximation, with no difference in treatment of saturated and unsaturated flow (Figure 6b). The flexible finite element formulation of the subsurface domain allows the inclusion of greater parameter and numerical approximation detail as appropriate, for example where known spatial heterogeneity is important, and where recharge/discharge features such as river channels occur. It is a quasi-three-dimensional model, fully detailed in the two-dimensional vertical plane. It includes a form of SVAT (Surface Vegetation Atmosphere Transfer) and is computationally coupled with hillslope runoff by infiltration-excess and saturation-excess and with channel flow. The IHDM's representation of variable saturation within a single calculation domain offers a relatively

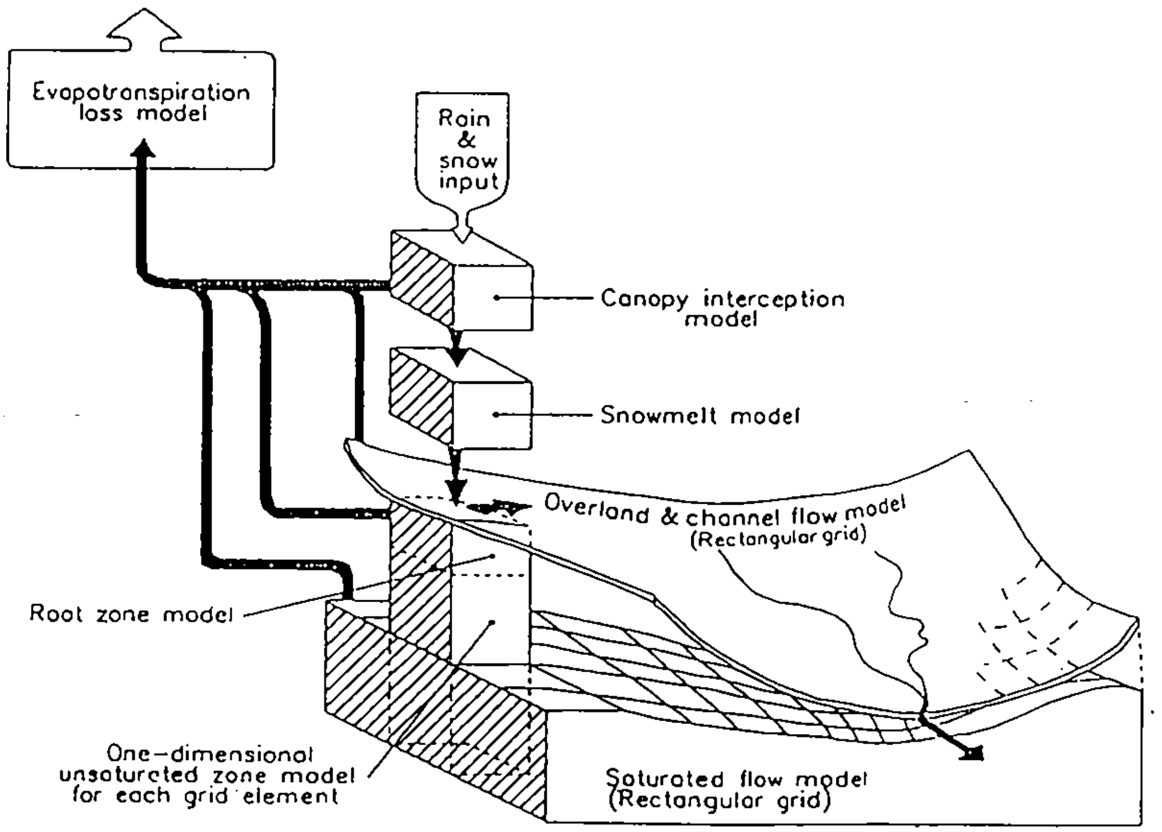
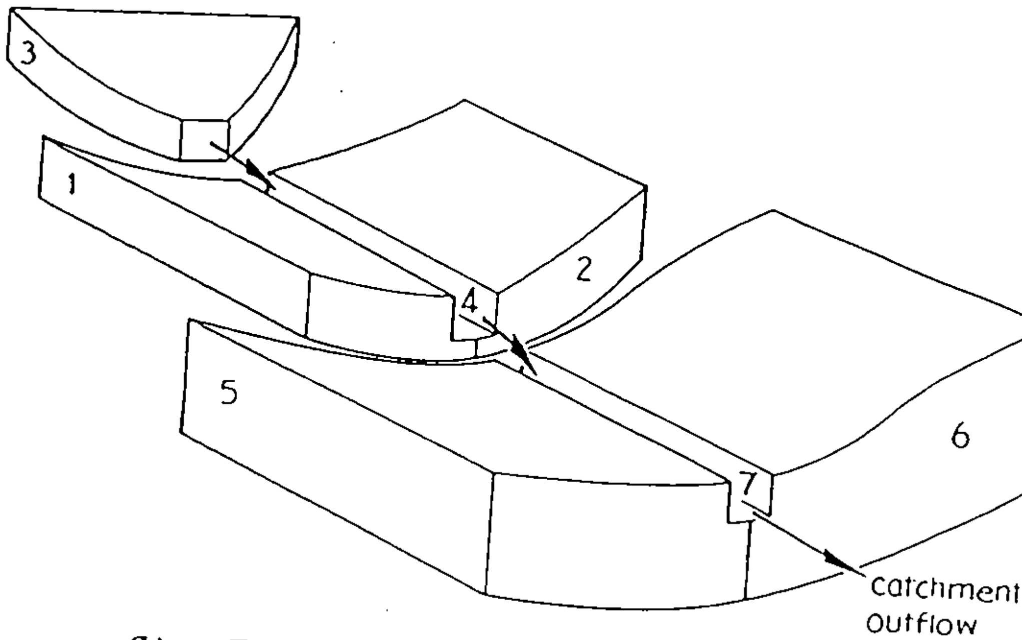


Figure 5 Schematic diagram of the Systeme Hydrologique European (SHE) hydrological modelling system

(a) Schematic structure of hillslope and channel components of the IHDM. 1, 2, 5, 6 hillslope component (sideslope); 3 hillslope component (headwater); 4, 7 channel component. Numbering indicates order of simulation of components.



(b) Example of a hillslope finite element mesh

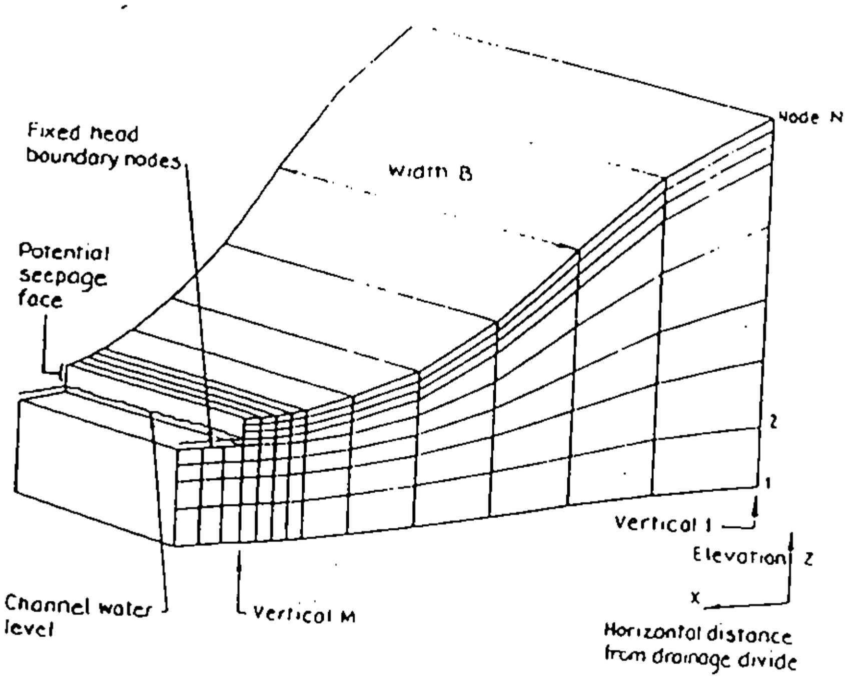


Figure 6 The Institute of Hydrology Distributed Model (IHDM)

straightforward way of handling perched water tables, in addition to fluctuating positions of saturated/unsaturated boundaries over time. At the same time it is possible to simplify the IHDM by reducing the grid detail and modelling catchments as a sequence of connected planes or segments. Figure 7 shows the increased level of detail moving from large catchment considerations through to small sub-catchments. The detailed river network data available at IH will be used as the basis of catchment models. Figure 8 shows the basic hydrological model at levels 1 and 2 in the figure forming the basis of a whole network of quality sub-models.

Within the LOIS programme it is therefore proposed to start with the IHDM structure. Hillslope elements will be identified on the basis of topography making use of the IH 50 m digital terrain data set. A simplified grid system will be employed such that the IHDM structure can be reduced in dimension. Detailed hydraulic properties will be estimated using extensive spatial databases available at IH. These include soil type, HOST (Hydrology of Soil type), Land Class, DTM etc.

The modelling strategy will be to apply both the full IHDM and the reduced order model (ROM) to a large number of sub-catchments and to validate the ROM as an acceptable flow simulation model. The ROM will then be applied to all sub-catchments of the East Coast rivers and sub-catchment models linked together in a network. Outputs from the ROMs will feed into the channel and groundwater models described below. The combined flow model will require sophisticated software and will require a LOIS supercomputer for full integration with chemical sub-models.

River Channel Model As shown in figure 5 a channel flow model is required to transport flow and pollutants from catchments to tidal limits. There are several approaches possible here from solving the St Venant equations for channel flow through to solution of ordinary differential mass balance equations. A modelling strategy which maintains a balance with the reduced order distributed model described above would be to use the continuity equations for flow along rivers.

Groundwater Modelling At large spatial scales, such as being considered under LOIS, groundwater is an important component of hydrological fluxes, since the likelihood of occurrence of (semi-) permeable strata increases, as does the occurrence of regions of recharge to and discharge from subsurface water systems.

Groundwater is important because of its great volume, albeit moving at low transfer rates: usable groundwater in storage is equivalent to some thirty-five years' runoff in the Yorkshire Ouse. In addition, an understanding of flow pathways and residence times of groundwater transfers can help explain hydrochemical fluxes.

To determine the primary inputs to groundwater systems requires knowledge of the spatial and temporal variations of ground surface fluxes, and the behaviour of water in the soil zone and any unsaturated zone beneath it. The groundwater systems in the Yorkshire Ouse and Yorkshire Ouse discharge to springs and the river channels. Within LOIS the University of Newcastle TRACE 1 model will be used to simulate major aquifer transfers to coastal systems. This model can simulate pollutant transport in addition to flow and can therefore provide flux estimates. Appendix 3 describes TRACE 1 in further detail.

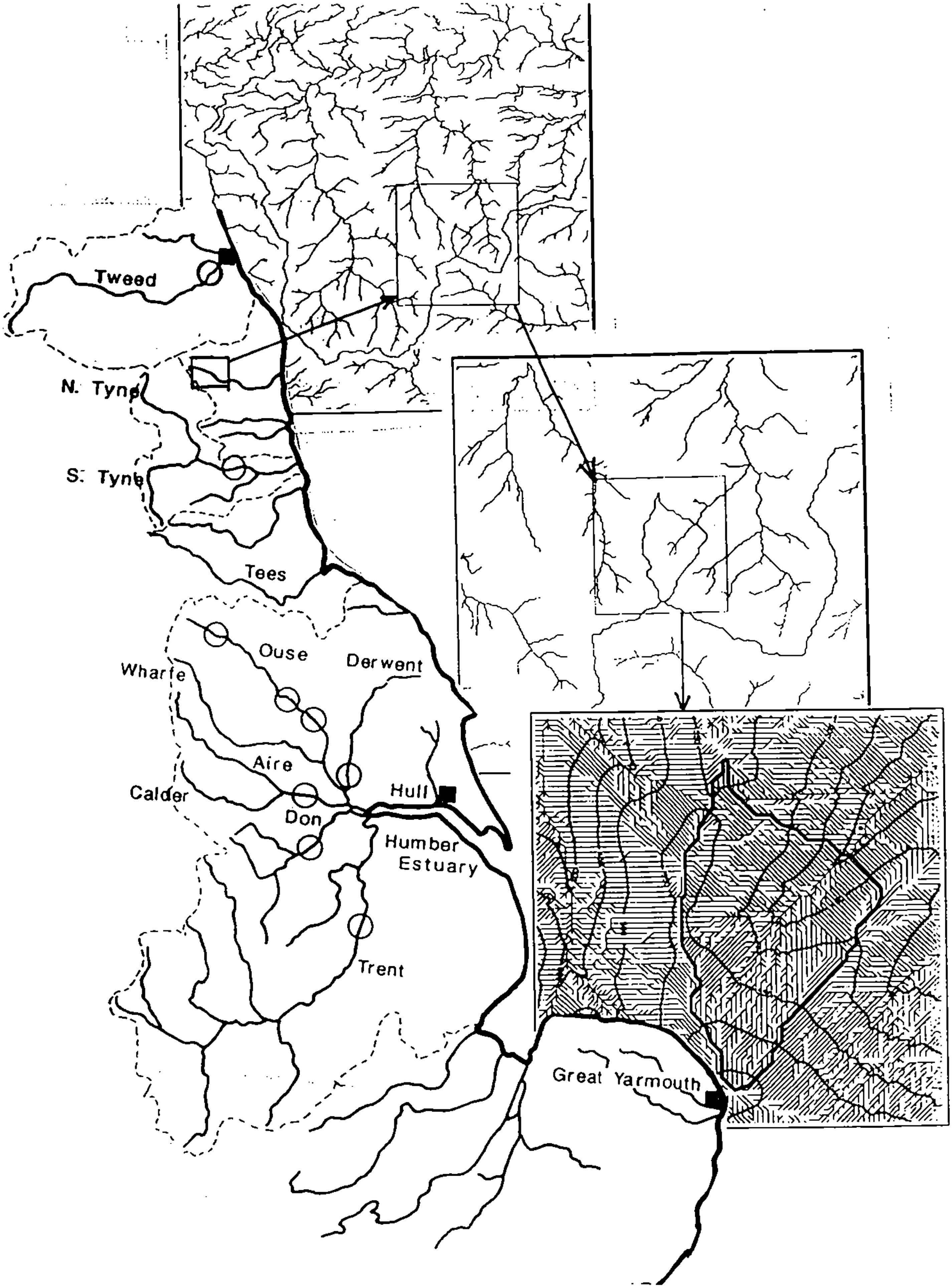


Figure 7 Catchment River Networks showing increasing levels of detail

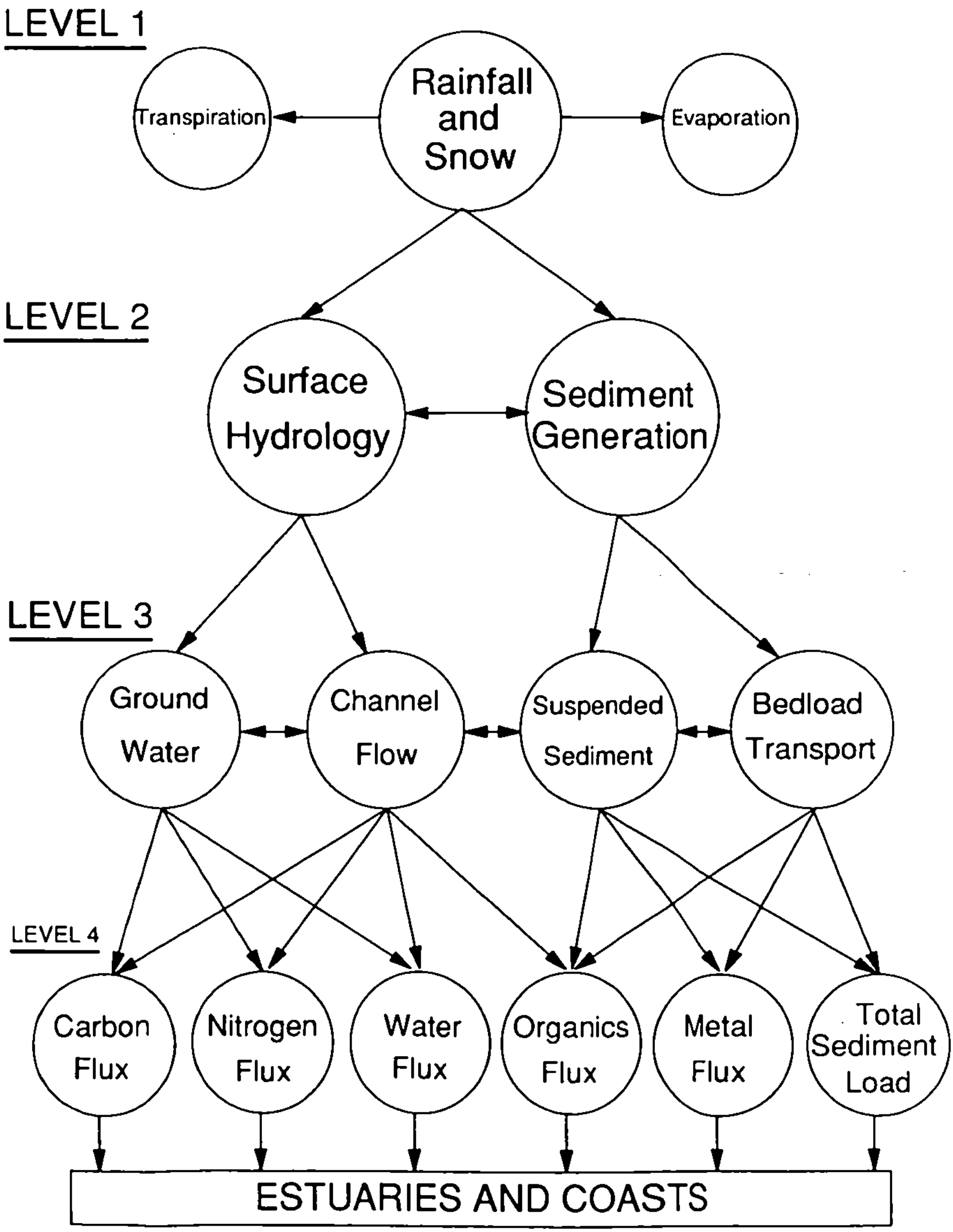


Figure 8 Sub-component models and interactions

4.2 Sediment Dynamics and Modelling for LOIS

The aim of the sediment modelling work in the core modelling programme of LOIS is the production of a time series of daily outputs of sediment from the East coast rivers over a range of time spans. Model output of bedload, suspended load and particle size characteristics will be required. As one of the uses of the model will be to assess the impact of land use change under different weather scenarios, it is important that the model is rooted in an understanding of the processes operating. It is also important that the short-term model should be compatible with long-term models being developed within the NORMS programme of LOIS and, therefore, extensive collaboration with other researchers is envisaged (see Figure 9).

The large spatial scale identified for the modelling work means that highly detailed process-based modelling over the entire river system is not possible. However, because of the relatively fine time scale, sufficient process detail needs to be incorporated to describe the behaviour of sediment over the course of a single storm hydrograph. The problem is, therefore, not a trivial one but requires the implementation of a model that will cope with the fine time scale within the context of a large spatial scale. The short time span, however, does have one advantage in that sediment movement can be considered as a function of the sediment supply and the existing hydraulic geometry of the river network i.e. the rivers can be assumed to be largely fixed over this time span. However, some fluvial adjustment, such as that following extreme events and adjustments in particle size distribution downstream and in the vertical, will need consideration in the model as a feedback mechanism.

The flow component of the model being used within LOIS will be able to provide hillslope flows, subdivided into surface (quick) and subsurface (slow) flows, as well as general water table depths within the slopes; and flow in all the river channels. The question of whether to route the flow through the river network "hydrologically" or using more detailed hydraulics will have to be addressed. In either case, the hydraulic details may still be insufficient to drive an adequate sediment transport model directly; hence the overall approach to the sediment modelling suggested below.

The strategy that is proposed is a hierarchical approach in which the river system is subdivided into reaches (about 1 km in length) which are classified according to their hydraulic and sediment characteristics (see Table 1 for more details). An example of each reach type would then be selected for detailed monitoring and the development/implementation of a detailed physically-based simulation model which would be calibrated and validated at the chosen site. The results from this model would then be abstracted to give a simple relationship between flow and sediment transport parameterized for the type of river reach. This would allow the significant processes for each type of reach to be recognised and incorporated into the large scale framework, albeit in a simplified manner. This is vitally important because of the poor performance of general sediment transport equations which fail to take into account details such as gravel-bed structure, sediment supply, and the nature of cohesive materials.

Sediment Modelling Details There are two aspects of the sediment transport modelling problem –

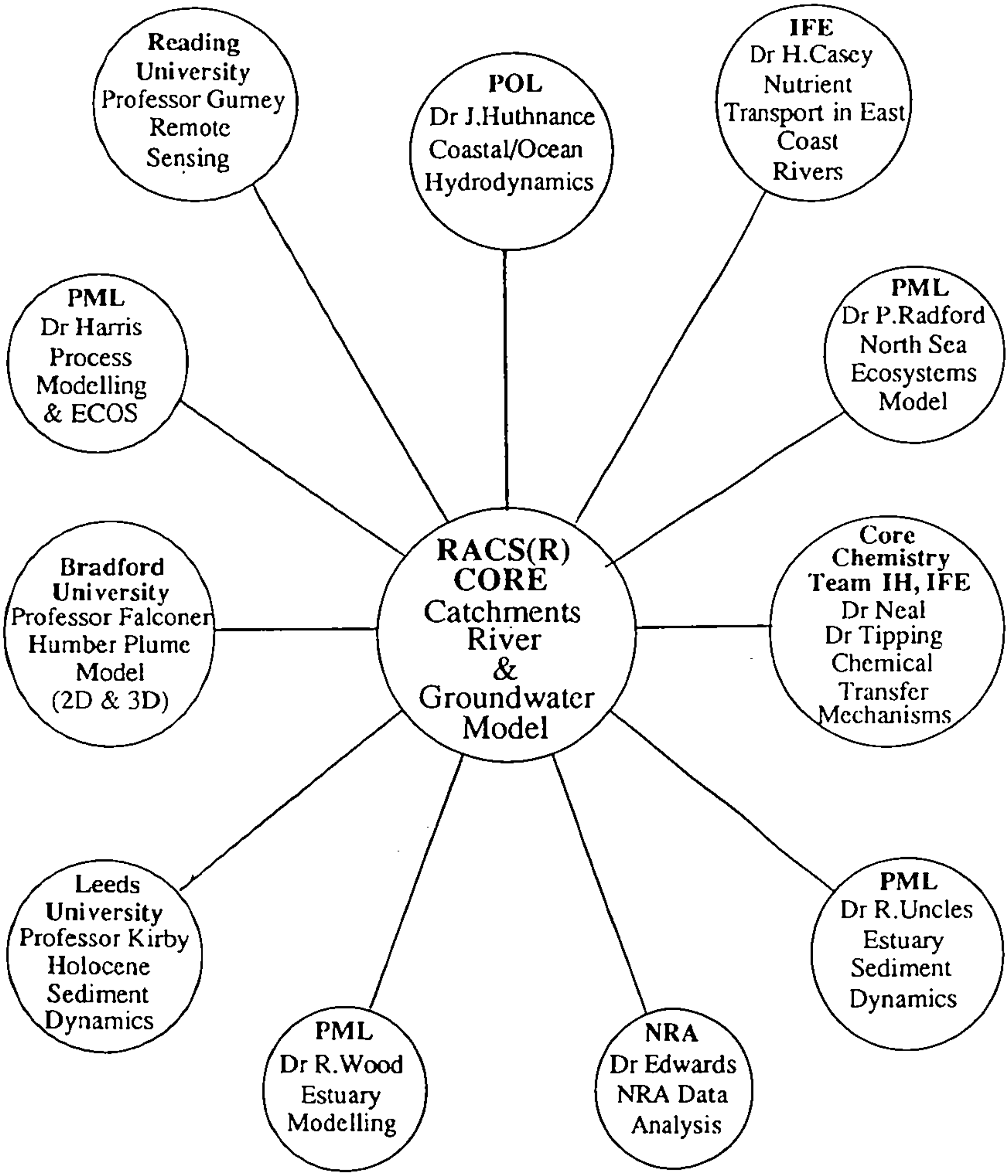


Figure 9 RASC(R) Core Modelling and LOIS Project Links

1. Delivery of sediment into the river system

2. Transport, storage and re-suspension of sediments within the river system.

Once suitable models for each of these components are derived for each of the different classes of river reach, then the large-scale model basically comprises a continuous sediment budget, by size fraction, for each reach down the observed river network. It is also apparent that sediments, metals and organic contaminants are closely linked via the adsorption of metals onto sediment particles and this link will need to be made with the water quality component of the core modelling programme. These aspects are considered in later sections of this proposal.

Table 1 River reach classification data

	Characteristic	Details
1.	Location Length of reach	
2.	Channel width Flood plain width	
3.	Hydraulic type	Boulder stream Pool-riffle sequence Sand waves
4.	Bed particles	Surface grain size (D_{50},D_{84}) Subsurface grain size (D_{50},D_{84}) Bed structure Cohesive materials
5.	Bank erosion	Rate (volume) Particle size distribution
6.	Landslide sources	Threshold Volume Particle size distribution
7.	Hillslope sediment sources	
8.	Sediment sinks	Reservoirs (trap efficiency) Rates of infiltration into bed sediments Presence/size of dead zones
9.	Contaminants	

4.3 Nitrogen Transport

Nitrogen fluxes are particularly important in rivers, estuaries and coastal ecosystems as N acts as the principal nutrient controlling eutrophication processes. The RACS (R) core model must therefore provide a comprehensive description of N-transport in catchments and rivers.

There is already considerable expertise in IH in developing nitrogen process models with catchment hydrology. For example, Institute of Hydrology Distributed Model for Nitrate Transport and Transformation (IHDMTRAN-N) has been developed for predicting water and reactive solute movement through one or more hillslopes, with linkage to an open channel or freely-flowing drain. It is derived from the IHDM by the addition of N transport and transformation. Processes are modelled using the conservation equations for flow through porous media and surface flow, coupled with advection-dispersion for solute transport, and N reaction chemistry in soil and surface water. The subsurface and surface components of the model may be integrated to give an idealised routing of water and N through a complete region. In practice, separate components of the model are suitable for use at different scales under normal restrictions on data availability. The subsurface components is suitable for use at plot scale, while the surface water component may also be used at a larger scale.

The principal forms of soil nitrogen are NH_4^+ and NO_3^-, organic-N and denitrified gaseous nitrogen species, with most solution phase N in the form of NH_4^+ or NO_3^-, but the latter is more prone to leaching. the model combines the simulation of single-phase fluid flow in partially or fully saturated porous media, with the reactive solute transport of the coupled nitrogen species NH_4^+ and NO_3^-, under the influence of specific chemical and physical transformations.

Temperature dependent biological transformation of the nitrogen species takes place, continually altering the distribution of N among its various forms. These transformations are further dependent on soil moisture and the concentrations of the other nitrogen species. A linked model simulates nitrogen species and temperature and this will form the core of the LOIS catchment once linked to the reduced order IHDM. Further details of model equations are given in Appendix 4

4.4 Carbon Fluxes

Studies of the fluxes of carbon to the oceans are important in relation to an understanding of the global carbon cycle (eg atmospheric CO_2 generation), acidity regulation within the rivers and environmental water quality impacts in the estuarine regime associated with particulate matter transfers and biochemical interactions.

The supply of carbon to the oceans comes from both inorganic and organic components. For the inorganic supplies, there is both a dissolved term ($H_2CO_3^0$, HCO_3^-, CO_3^{2-}) and a particulate component associated with transport of sediments (eg $CaCO_3$ form carbonate bearing bedrock). For the organic supplies, the carbon fluxes split into two components (1) the component which passes through a 0.45μm filter, the dissolved organic carbon (DOC), and (2) the component retained by a 0.45μm filter, particulate organic carbon POC).

For dissolved inorganic carbon (DIC), the bicarbonate and carbonate concentrations increase in
response to increased mineral weathering and agricultural activity such as liming. Carbonic

acid increases as biological activity increases due to the higher pCO_2 levels and this too can lead to higher DIC concentrations. Assessment of the inorganic carbon levels is important in relationship to determining the extent of acidity regulation within surface waters and this has a bearing on other aspects of the chemical modelling work (eg solubility controls for the heavy metals).

For organic carbon, the composition of river waters represents a complex series of compounds. Many of these compounds have still not been categorized fully and the processes regulating them have not been adequately established. Within a modelling programme there is very limited scope for dealing with the fate of the individual compounds owing to the uncertainty and complexity of processes involved. Never-the-less a valuable contribution to the overall LOIS objective would be to try to model the gross changes involved.

In many lakes, small streams and in the open ocean, POC concentrations are less than 10% of the total organic carbon (POC+DOC), although in larger rivers and for smaller catchment areas where land disturbance has occurred POC may be as large or even larger than the DOC fraction. With increasing discharge POC increases dramatically while DOC changes less. Generally, the combination of primary production of plant matter and decomposition rates determines the amount of DOC in water although of course hydrological factors come into play when determining short term and seasonal variations: climatic factors may also be of importance for example water treatment problems associated with increased colour has occurred within recent years. Particulate organic carbon is typically 2 to 4% of the sediment load and it is determined by the vegetation type, geology and the seasonal variation control of the percent organic carbon in the suspended sediment. Organic matter from land (eg plant and woody materials) are diluted by minerals and clays especially when erosion rates are high. Also, POC originating in rivers (eg plankton production) is diluted by mineral sources from the land. Moreover, with increased sediment load, primary production is reduced due to decreasing light penetration into the water. All these processes work towards decreasing the proportion of POC in the sediment, with increasing sediment concentration. Times of travel for POC in rivers varies down a basin and for lowland rivers the stores may well remain for upwards of a 1000 years. Thus POC undergoes a very different history than DOC.

For some estuaries, the DOC is chemically conserved and there is a linear relationship between DOC and salinity. DOC concentrations in sea water are lower than in the freshwaters and the further out to sea the lower the DOC levels. For other estuaries, DOC behaves non conservatively and this may well be associated with the flocculation of the colloidal materials in the river water due to the higher ionic strengths met in the estuary. The amount of DOC lost from solution by such processes can typically be of the order of 10%. Within the estuary there may be a source of DOC associated with biological conversion of POC which is a function of the chemistry of POC. There are processes such as eutrophication that increase the concentration of both POC and DOC, particularly at the seaward edge due to upwelling of nutrient rich waters. Within the estuarine and marine bottom sediments, a complex series of sedimentological, hydrodynamical and biological processes determine organic carbon levels.

Within the RACS(R) core modelling project a 'global' carbon balance model will be produced in which the major sources of carbon will be identified. Links with the hydrological and sediments model will be required but an overall mass balance approach may be possible. Biological components will play a key role and interaction with scientists at the Institute of Freshwater Ecology will be required. Models such as the algae growth and transport model described in Appendix 5 will be used to simulate biological components.

4.5 Heavy Metals Transport

Heavy metals are of great significance to coastal ecosystem because of their toxic nature and their impact on aquatic flora and fauna. The major sources of metals in rivers such as the Yorkshire Ouse and the Humber will be from direct discharges of industrial and domestic effluents. The prediction of these will require information on discharges and thus collaboration with the National Rivers Authority will be essential.

Heavy metals modelling has been undertaken at IH on rivers such as the River Pelena in South Wales and the approach has been to provide a mass balance and assume minimal transfer between particulate metals, adsorbed to sediments, and dissolved metals in the water column. In fresh water environments in large river systems this assumption is acceptable for certain metal species such as iron, nickel and zinc. However, for others such as aluminium and cadmium, the transfer processes are significant and metal speciation is complex. Within the core modelling programme the model QUASAR (see Appendix 6) will be used initially to establish overall mass balances for metal transport and where necessary this model will be extended to link with sediment transport models.

In river systems not heavily impacted by effluents natural processes will control the heavy metal balance. For example, acidification will be a major driving factor controlling aluminium release and land use change such as afforestation and deforestation will exacerbate this situation. Many of the processes controlling metal release have yet to be fully understood but models such as MAGIC (Model of Acidification of Groundwater in Catchments) provide a basis for simulating long term changes in atmospheric pollution and land use (see Appendix 7).

4.6 Organics

Another area of concern with RACS(R) and LOIS is the transport of organics into coastal ecosystems. As in the case of metals, organics are often discharged into rivers from industrial sources and a QUASAR mass balance approach linked to the sediment transport model would be appropriate for these discharges.

Many organics are derived from non-point sources such as agrochemical runoff draining field systems. This is a much more difficult area of modelling because of the vast array of processes that control organics transport and distribution (see figure 10). At IH a simplified catchment model has been established and details of this together with an application is given in Appendix 9. The model described will be expanded as part of the core modelling programme and linked to the hydrological model described in Section 4.1.

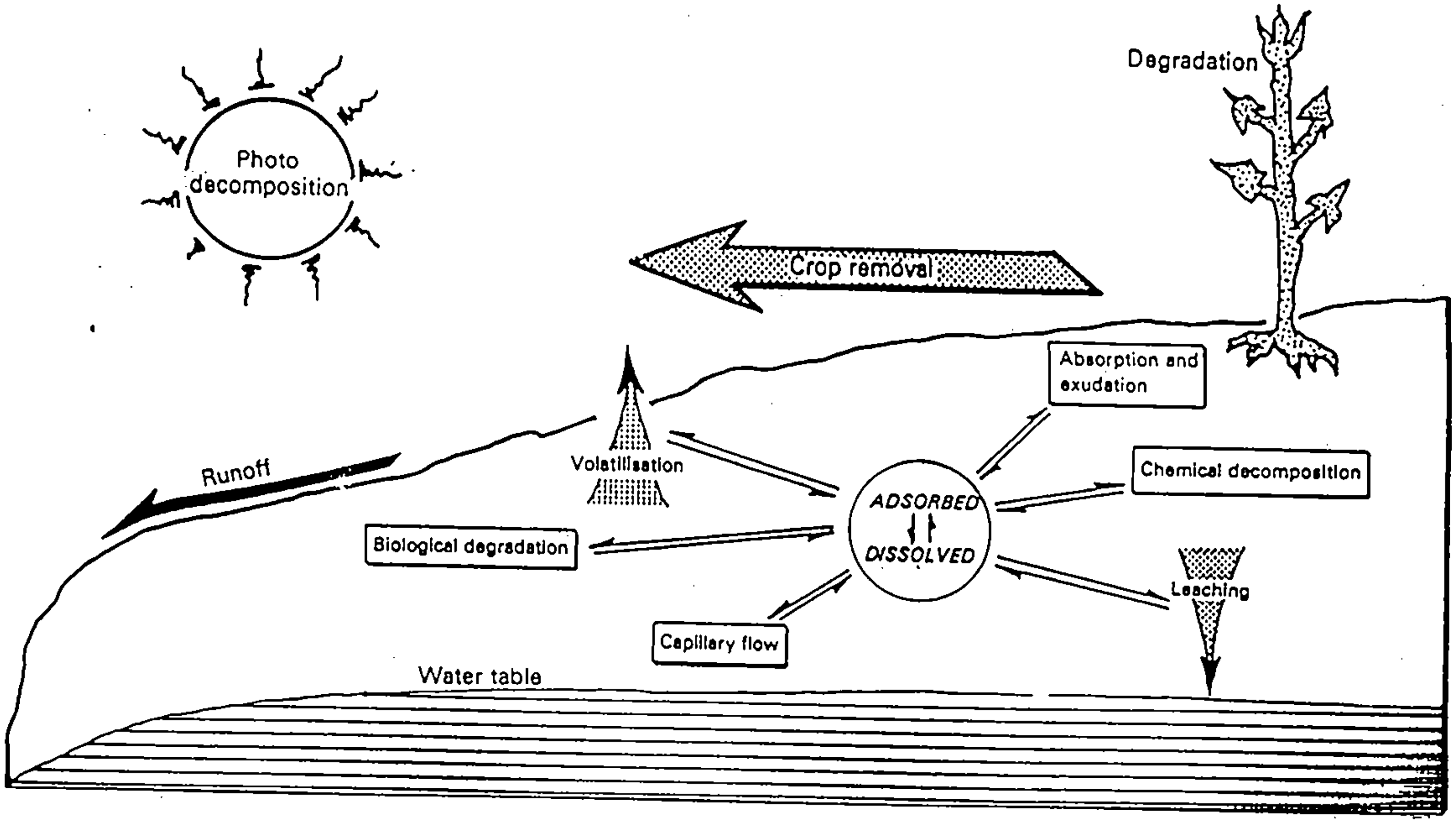


Figure 10 Processes influencing the behaviour and fate of pesticides in the soil environment (redrawn and modified from Weber et al., 1973).

4.7 Linkages Between Sub-models

Figure 8 shows the principal linkages between the sub-models. Distributed flow models drive river channel models and also interact with sediment and chemical constituent models. There are many feedback processes operating in catchments and, in addition, processes are highly non-linear. It is imperative that an advanced modelling structure is established from the outset so that model integration problems are minimised.

5. SCENARIO STRATEGY AND LINKS WITH OTHER LOIS PROJECTS

The whole rationale of the LOIS programme depends on being able to model historical behaviour of catchments, rivers and coastal ecosystems and then to run these models forward to predict the likely impacts of environmental change. Such changes include differing climate scenarios, varying land use patterns, changing atmospheric pollution levels and direct pollutant impacts from industrial, agrochemical release on domestic effluents. Detailed scenarios will be discussed with other members of LOIS projects to ensure LOIS objectives are being fulfilled.

As part of the RACS and NORMS implemented plan (see Appendices 1 & 2) detailed scenario runs are envisaged. Daily (and more frequent) time series of flow, sediments and chemical constituents will be provided to coastal and estuary modellers for all the key scenarios. Because of the considerable interactions between the different model components, substantial computing power will be required (see Appendix 10).

Generalised Sensitivity Analysis The techniques of generalised sensitivity analysis (GSA) have become established in recent years as a powerful tool for analysing complex dynamic interacting systems. GSA was first developed by Hornberger and Spear (1989) in a major catchment - estuary system in Western Australia, the Peel-Harvey Inlet. The aims of the Peel-Harvey study were very similar to LOIS in that the land surface coastal ecosystem interactions were studied to determine processes controlling ecosystem change. The GSA techniques will be used extensively in the RACS core modelling project to assist in model formulation and the identification of key parameters and processes.

Links with other LOIS Projects The RACS(R) core modelling project is fundamental to LOIS as it is impossible to realize the aims and objectives set out in the LOIS science plan without an integrating technique for translating catchment inputs and changes into catchment outputs - such outputs provide the key driving variables for the estuary and coastal ecosystems models. Figure 10 shows the principal research groups involved in direct collaboration. This figure gives an indication of the wide range of expertise that will be utilised within LOIS and more importantly the large number of groups that will be dependent on the results of the core modelling programme.

6. DATA COLLECTION, ANALYSIS, GIS AND WIS

Appendix 9 gives details of the data centre to meet the needs of RACS. This data centre will contain time series chemistry, hydrology and meteorology for the East Coast rivers.

In addition it will hold extensive spatial databases such as the digitised river network, HOST (Hydrology Of Soil Types) and land use data. With these data it will be possible to establish dynamic models and take into account spatial variability. The GIS system ARCOINFO will be used to manipulate spatial databases and the IH Software System WIS will be employed to manage the total database.

These data management techniques will provide a powerful tool for model development. Also they will provide a means for other LOIS researchers to access data and model simulation results.

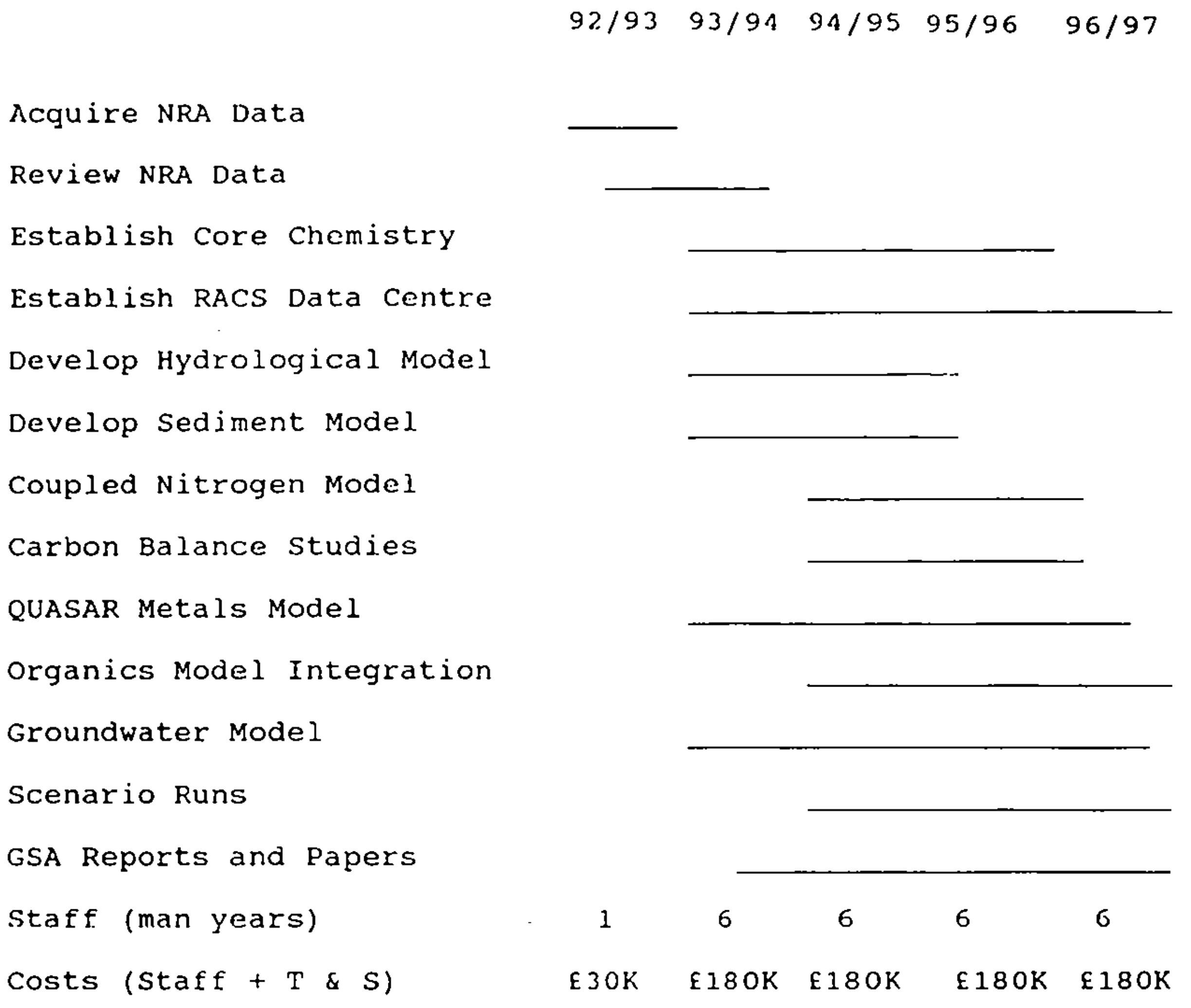
7. DURATION, STAFF LEVELS AND COSTS

Figure 11 shows a bar chart giving the principal activities involved in the core modelling project. It is envisaged that modelling studies will start this financial year and will continue throughout LOIS until 1997.

The total costs of this programme of research will be £30K in the current year and £180K per annum thereafter which was agreed at the RACS(R) Committee Meeting in June.

8. COMPUTING

The models developed from the core programme will be run on a range of hardware including Unix Workstations and a LOIS supercomputer facility. Details of the computing requirement are given in Appendix 10. It is essential that a LOIS machine is available at Wallingford for detailed model development.



TOTAL COST £750K

Figure 11 BAR CHART OF RACS(R) Core modelling project

APPENDIX 1

RACS RIVER BASINS - SUMMARY OF OUTLINE IMPLEMENTATION PLAN

OBJECTIVES

The three main aims of the river basins research within LOIS are stated in the Science Plan. These are:

1) To determine contemporary land-sea fluxes (of water, sediment, biological matter, major dissolved constituents, nutrients and contaminants).
2) To identify and characterise key processes governing the flux.
3) To develop models to predict flux resulting from future changes (eg. in land use or climate).

These aims should remain the same within the implementation plan. A reassessment of the detailed objectives, themes and spatial coverage has led to the following recommendations for prioritization and modification.

Priority measurements and themes
The Rivers Basins subcommittee has considered the core activities listed in the Science Plan. All elements of the core programme listed in the Science Plan are recommended as essential to the LOIS Programme. With regard to the thematic activities, the following topics are selected (in priority order):

1) Top priority is given to fluvial sediment dynamics and processes, the biology and chemistry of nutrient cycles and riverine carbon fluxes.
2) Particle-solution partitioning of contaminants and nutrients.
3) The hydrological processes which determine movement of water and the flux of many other substances and the associated interactions between the physical, chemical and biological systems.
4) The influence of dead zones was not given high priority with regard to the large river systems of the Humber catchment, but may be of some relevance in the Tweed system.

The land use impacts heading may be important within the RACS context (early indications are that this may be a responsibility of the DATA component committee). There is a pressing need for preliminary field and archive data collection in the core study area.

Spatial Priorities
With regard to the study sites, the primary focus should be upon the Yorkshire Ouse. The other principle rivers contributing to the Humber will be covered by single monitoring stations in the lower reaches. In some cases there is a need for the establishment of ultrasonic gauging at the river/estuary interface, mostly for short term deployments (often associated with intensive estuarine studies). In the Yorks Ouse there will be a long-term Ultra-sonic primary station established, probably at Nabum Weir between York and Selby. The river fluxes to the Humber estuary are very complex. There is a multiplicity of major rivers with large scale water transfers and effluent inputs. The Tweed has been chosen as the other area of intensive study, because of its contrasting characteristics. Tweed studies should be approximately 20% of the activities of the LOIS River Basins Sub-component of the programme. There is a need for close links with NRA regarding both data and facilities.

Core and thematic programme objectives.
Physical Sediment Studies - The magnitude and timing of the flux of sediments needs to be quantified in the study rivers. The core programme should provide good quality data for the primary gauging stations, principally of fine sediment loads. This will be collected on a routine and event-related basis. Estimations of particulate flux will be required for each basin

within the core study area. In order to understand sediment transport and to predict potential impacts of future climatic, land-use and other changes, investigations into sediment sources, conveyance and sinks will be required, although the emphasis in this work should be at a 'basin-wide' scale.

The core and thematic work will be closely linked, eg.much of the sediment sourcing work would be outside the core programme activities (which will be mainly concentrated upon the primary stations). However, samples of particulate sediment load will be made available from the core study for thematic work. In addition to the quantity of sediment flux, attention should be given to the characteristics of sediment being transported, such as particle size and mineralogy, and how such characteristics are affected by transmission through fluvial and estuarine systems. A proper understanding of 'freshwater' and 'saline' particle aggregation processes will be vital in this regard. There will also be a need to place current sediment fluxes into a longer term context involving the reconstruction of sediment yields in the recent past (last 50-200 years). Close links with LOEPS are required.

Chemistry and contaminants - The core work will mainly be the chemical sampling and analysis, to determine fluxes and budgets. The chemical conditions in the rivers will also need to be defined to underpin process studies. The following groups of determinands will be considered; major ions, pH/conductivity/oxygen/temperature, trace metals, nutrients, carbon, organic micropollutants.

The understanding and prediction of chemical fluxes requires investigation and characterization of a number of key processes. To achieve this, thematic studies on the following topics are needed;
1) Chemical processes involving particulates. The incorporation and release by suspended and sedimented particulate matter of nutrients, trace metals, organic micropollutants and tracer chemicals need to be characterized and quantified.
2) Chemical modelling, to include solution-phase speciation and particle uptake/release, in order to predict the chemical forms and availabilities of chemical components at different points in the river system.
3) Collaboration between chemists and biologists on the role of biological processes in determining the sources, fluxes and fates of nutrients and micro-pollutants.

River Biology - Biological studies will be conducted almost entirely on the Tweed and tributaries of the Humber, although sampling may be needed from other rivers to provide information essential for coastal or estuarine LOIS studies outside these catchments. In order to make effective use of resources, the most detailed studies should be made on the Ouse and its tributaries and the most intensive period of sampling should be conducted in 1995. The core programme will be concentrated upon collection of routine, seasonal and event-related data at primary stations (eg. on phytoplankton and macrophytes) in addition to linkage with chemical and particulate fluxes.

The aim of the thematic biological programme will be to identify and quantify the key biological processes influencing the flux of major elements within the rivers, especially oxygen, carbon, nitrogen and phosphorus. The studies will be concentrated on downstream sites as far as the freshwater/saline transition zone. The various processes should be investigated in both the water column and bottom sediments. There will be a requirement for taxonomic and general ecological studies, where this information is essential to understand the processes influencing nutrient flux or to assess information about long-term changes from sediment cores or historical records. There should be close collaboration between the various investigators, especially during the year of intensive study (1995).

Integrated Modelling - The third aim of River Basins research within LOIS is to predict future fluxes. The objectives of the modelling should be: to identify the catchment-scale hydrological and other controls upon flux of water and associated materials to channels; to understand the processes controlling the behaviour of key water quality determinands, sediments and biological systems; to assess land use and climate change impacts upon river flows and water quality; and lastly, to provide simulated daily/hourly data for river flow and water quality from river to estuary/coastal systems. Model development within individual process studies should be combined with channel and distributed models to produce an integrated model which links spatial and temporal databases, within a GIS format, compatible with model development in the estuaries and coasts component of RACS and NORMS.

TIMETABLE

Year 92/93 93/94 94/95 95/96 96/97

Prelim. work

Core Programme
Fieldwork
Lab. analyses
Data management
Intgr. modelling
Tweed (SCAT)

Thematic Programme
Process studies
Cont.
Episodic

SPREADSHEET (£millions)

a. Core activities	-	3.291
b Capital	-	1.53
c. Thematic activities	-	1.0
d. Computing	-	0.4
e. Field op (Gauging Stns).	-	0.465 (incl. within b.)

RESOURCES

The following resources are required mainly for use in the core programme. However "joint access" will be organised with Special Topic project teams, where significant cost savings can be made.

		£k
Flow gauging equipment	-	500
Water Quality sampling network	-	210
Sediment monitoring network	-	195
Logging system	-	60
Portalab	-	70
Field transport	-	40
Boats and trailer	-	45
Field lab/offices1	-	230
Main analytical facilities	-	195
Contingency equipment for Year 3	-	150

LAND-OCEAN INTERACTION STUDY (LOIS)

"INSTITUTE SUPPORT" FUNDING WITHIN THE TERRESTRIAL AND FRESHWATER SCIENCE DIRECTORATE

A - DISTRIBUTION OF FUNDING UNDER "INSTITUTE SUPPORT".

The following table shows the provisional breakdown of work under the "Institute Support" heading based upon the likely funding of TFSD work of £450,000 per annum.

Activity	% of underpinning funds
Operational management	15
Data base management	9
Fieldworkers based near river basins core site	30
Chemical analyses	19
Coastal work	11
Instrumental back-up	7
Contingencies	9

The money available does not cover the full programme of work which will be required from institutes, however funding will be used to cover a large part of the core programme activity.

B - LOIS-RELATED WORK IN TFSD

In addition to full use of the underpinning money for LOIS support, there are 75 major projects within TFSD institutes which are related to LOIS. These range from field-based studies on rivers and coasts, process studies, analytical work, modelling and development of GIS systems. Not all of the acties within these projects are fully relevant to LOIS. However, it is estimated that approximately £5.5 million per annum of this work is directly related. The resources of expertise, equipment, software and data archives from these research projects will provide significant additional support for the LOIS programme at no additional cost.

C - TFSD LOIS OPERATIONS

A two-fold division can be made in the location of personnel, between existing institute sites and those based close to the core study site. Their possible roles are defined below:

The field scientist team

This will be a group of five to eight TFSD scientists. It is anticipated that there will be hydrologists, geomorphologists, chemists, river biologists and coastal ecologists. They will be concerned with the field operations associated with the core programmes. The work will include:

a) Assisting in the installation of monitoring facilities,
b) Carrying out routine and event-related sampling,
c) Maintaining the flow gauging, bulk sampling and continuous monitoring networks.
d) Feeding data to the main LOIS computing facilities, following initial quality control.
e) Some full laboratory analyses and preparation of samples for further analyses at the main Institute bases or HEI's.

The team will be augmented by additional staff during intensive sampling campaigns and during specific Special Topic work (which should occupy 20% of their time). The main base for this team will be within the Yorkshire Ouse catchment at Riccal, near Selby, or York. A large part of their time will also be spent at the likely lab and office facilities at Hull University, for access to workstations and additional analytical facilities. The coastal ecologist may be mainly based at a location more closely adjacent to the Wash and N. Norfolk.

During year 1, in addition to installation of equipment, calibration of instruments and reconnaissance sampling (eg. during flow events), the team will be involved in the trawl of archive data and background literature on the core study area.

Main Institute activities

These will include:

a) Most of the chemical analyses for substances which do not suffer from storage, transportation requiring the use of analytical facilities which are (or will be) available at IH, IFE or ITE. Similarly, some biological analyses will be carried out at IFE and ITE.

b) Remote sensing work will be instigated and outputs processed and interpreted using the existing TFS facility at Monkswood.

c) Data management including archiving and incorporation of data from field, labs, remote sensing and external sources (eg. NRA) in to GIS system and two-way links with Bidston. This will be focussed upon IH, Wallingford, given high speed links with Bidston, but with dedicated LOIS workstations in the core study area, IFE, Windermere and ITE, Monkswood which will contain frequently updated core programme data.

d) Modelling activity - Catchment modelling activities to produce flux estimates will be based at IH Wallingford. This will be an essential part of the core programme but can not be funded from the "institute Support" category as it stands.

e) Instrumental back up will be provided from the appropriate main institute dependent on where the appropriate expertise is available.

APPENDIX 2

NORMS - draft implementation plan - June 1992

1. Objectives (in priority order)

1.1 Water-quality models, shelf-wide with appropriate land and ocean boundary conditions, embodying hydrodynamics and non-conservative constituent behaviour; specific example constituents to include a nutrient, trace metal, a land-ocean flux tracer and an organic pollutant.

1.2 Geomorphology: models addressing decade-to-centuries evolution with a coastal focus (extending offshore as far as the involved sediment transport, and alongshore from eg. Flamborough Head to Norfolk) assessing the impacts of sea level, storm frequency, rainfall, freshwater, land use,...through scenarios spanning the past eras of measurements, documentation and post-glacial records.

1.3 Buffering of fluxes of the same water quality variables received from catchments from the Tweed to the Wash, in the estuaries and a coastal strip including the interacting outflow plumes (eg. Humber-Wash; a RACS objective), to be modelled for a range of scenarios representing changed conditions over the last 200 years (the specific NORMS aspect).

1.4 Later carbon cycle (ecosystem) models with scope similar to (1.2) *geomorphological models* according to systems studied in RACS (coastal) and addressing questions such as *What is the impact of land-derived nutrients on the offshore ecosystem?* and *Given the rate of sea level rise, what is the rate of spread of X?*

1.5 To model the changing tides, patterns of shelf-sea stirring, sediment transport paths and hence evolution of the shelf system in response to Holocene changes in sea-level and glacial rebound (an objective shared with LOEPS).

1.6 To construct shelf-sea budgets with the shelf-wide models as an integration of RACS and SES (a corollary to the *Water Quality* objective 1.1).

1.7 The development of management tools should be the subject of commissions from responsible authorities.

2. Programme (numbering 2.1 to 2.7 corresponds to 1.1 to 1.7 in *Objectives*)

2.1 Water Quality

Constituents: u,T,S (necessarily as part of the physical transport model): other constituents to total about 10 including at least one nutrient (probably nutrient or total N); at least one trace metal (possibly Cd) and at least one organic pollutant chosen for availability of data, to be arranged through RACS if necessary. Primary production would probably be modelled to estimate sources and sinks of N, and effects of filtering organisms need to be represented for some metals and organic compounds. Sediments must be modelled in view of their role in transporting many constituents; there must be representation of erosion, settling, deposition, consolidation which may entail wave- and turbulence-modelling; particle-size distribution and different densities, organic fraction and partitioning between dissolved and particulate fractions of water quality constituents must also be modelled. Impacts of toxins (eg. on filtering organisms) are an appropriate subject for commissioned research, but the model should be extensible to accommodate them through a generalised organism model and at a population level (sedentary adults and planktonic larvae).

shelf-wide: a 3-D, ~ 3 km resolution hydrodynamic model (B-grid) (eg. extension to 60°N of a POL 3 km resolution prognostic 3-D 20-level model already in progress for the southern North Sea); acceptance of freshwater inflows and surface heating; develop a suitable representation for mixing (eg. through a prognostic turbulence kinetic energy equation - POL); incorporate transports and source-sink terms for constituents.

shelf-edge: prognostic 3-D 1 km resolution: investigate open boundary conditions, density/bathymetry representation for balanced pressure gradients, lack of numerical diffusion, parametrisations of turbulence, high-frequency internal waves and mixing; implement in 56-57°N × 8½-10½°W within shelf-wide model; incorporate transports and source-sink terms for sediments and ~~constituents~~ (chemical and biological processes - eg. 7-component plankton/nitrogen model, particulates, exchanges with sediments).

nearshore: 1 km resolution in an area at least 100 × 30 km off the Humber-Wash as in RACS(C), with characteristics otherwise as the shelf-wide model and embedded therein.

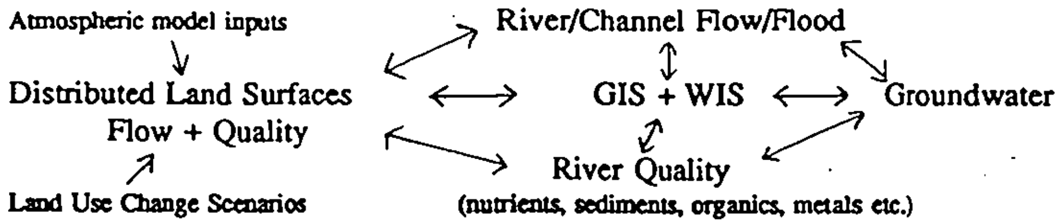
Input data needs are: meteorological forcing, initial temperature and salinity fields (assimilated to dynamical balance), river flows, groundwater flows, oceanic boundary values, sediment distribution and its size distribution, sources of modelled constituents, fluxes to/from sediments.

Validation data is available from the North Sea Project, and from POL current profile measurements for the shelf-wide hydrodynamics. Additionally, 1982-3 CONSLEX data and a semi-analytic model for wave forms will be used to verify the shelf-edge prognostic physics model. Needs from other sources (ICES and NRA to be investigated): organic constituents; finely-resolved data to correspond with the model resolution (aircraft - CASI scanner - and satellite remote-sensed data are envisaged for sea-surface temperature, phytoplankton pigments, dissolved organic matter). RACS will provide information for some prognostic constituents, guiding the choice of constituents.

Sensitivity analysis will be appropriate in several respects. Concentrations (of productivity, for example) at interfaces suggest the importance of stratification and mixing diffusivities, and hence a need for studies of sensitivity to values thereof. Other potentially important or poorly-defined quantities calling for sensitivity studies are sediment erosion thresholds and rates (affected by biota), sediment size distribution and organic fraction, toxicity in relation to binding, filtering by organisms, dissolved-particulate partitioning ratios and rate constants, the contribution of episodic events.

2.2 Geomorphology

catchment/river: models developed in RACS(R) will be used. These are shown schematically:



Databases are available for land use, etc. RACS(R) use extends to running catchment scenarios. However, application is needed to all catchments from the Tweed to the Wash.

coastal strip and estuaries: the model will be developed in RACS(C) (but all estuaries are needed) to represent u, density (including sediment stratification in estuaries), SPM. Resolution will be ~ 1 km, covering at least 100 × 30 km in 3-D (10-levels, say) and altogether extending offshore to include sandbanks. Evidently sediment transports must be modelled, invoking processes of erosion, settling, deposition, possibly consolidation modulated by size distribution, organic fraction and biological effects. As inputs to coastal sediment processes, tidal- and surge-currents, wave fields and wave-current interaction will be modelled. A wave-spectrum model is available (eg. WAM) for use to ~ 1 km offshore; then inshore wave transformation will be used. Initially, some parametric representation of coastal transport as a function of conditions may be appropriate. Tidal state may be the dominant condition in estuaries.

shelf-wide: a 2-D wave-surge-tide model is wanted; 12 km resolution should suffice. Such a system is expected to become operational in 1994 (POL & Met. O.)

Scenarios. "Time slices" corresponding to LOEPS data and different previous rates of sea-level rise will be run. A wave/tide/surge shelf model will be run offline for different tide, surge and wave scenarios, as outer boundary conditions for the coastal strip model. The scenarios will correspond to past climates and paleobathymetry (different sea level, glacial rebound using crustal model input from LOEPS, eg. Durham, and LOEPS core data, eg. BGS). According to wave model development for inshore sediment movement, the secnarios will enable estimation of the contribution of episodic events (fluxes from land and due to storms offshore. In the North Sea, it is estimated that 75% of transport is by episodic events).

Input data needed are: relative sea level, glacial rebound; LOEPS core data providing palaeogeographic maps of each of the major estuaries (for example) for sediments - implying definitive input in year 3 or 4 of LOIS. 1.6 may interpolate this input.

Validation data will include cores indicating palaeotides, sediment accumulations (land-based data for these are good, BGS cores exist offshore - some are commercial-in-confidence now but will be available - but there are very few nearshore in < 20 m and the LOEPS programme is needed).

Sensitivity to bathymetry needs to be assessed as a guide to the accuracy needed in the bathymetric reconstruction. Limits to predictability need to be addressed. The whole exercise is in effect a sensitivity analysis.

2.3 Estuarine Buffering

Constituents will be as for *Water Quality* and according to input and test data available.

catchment/river: model as in *Geomorphology*.

coastal strip and estuaries: the model will represent u, density, S, SPM and solutes as for *Water Quality*. (UK rivers are strong deliverers of contaminants and nutrients rather than sediments. However, estuaries are major stores and sinks of all these; and the Humber is very turbid). Resolution will be ~ 1 km, covering at least 100 x 30 km in 3-D (10-levels, say) and 400 x 50 km (Tweed to Wash) altogether. There may be stratification by sediments in estuaries. This will be developed in RACS(C).

shelf-wide: a 2-D surge-tide model with 12 km resolution should suffice, eg. the present operational model (POL & Met. O.)

Shelf-wide *scenarios* will be run off-line for the tide and surge as open boundary conditions for the coastal strip. Likewise, catchment scenarios will be run off-line for upstream inputs to estuaries, especially for times during the last 200 years when pollutants in rivers and estuaries have been important. Then there will be extended runs (months-years) for the relative contribution of "events" and the impact of changed conditions. These runs of the *coastal strip and estuaries* model will take as boundary conditions (i) catchment scenarios with average tide/surge (ii) tide and storm scenarios with average inputs from catchments. (ECoS is an existing simple and quick means of running scenarios, but needs extension for this purpose.)

The NELUP project experience with the Tyne catchment provides good experience on which to build this study, integrating ecology, hydrology and economics into a GIS (contacts Prof. Gurney, O'Callaghan, Ann Roberts TFSD).

Input data needed are historical rainfall and land use for the catchment model (from RACS(R), LOEPS), offshore tides and surges as above, past (estuarine) bathymetry form LOEPS cores etc., and past contaminant inputs from the NRA *via* RACS(R) (same range of variables as for *water quality*).

Validation data are needed *via* RACS(R) and LOEPS: past and LOIS cores, salinity records, ^{210}Pb (available with a peak ~ 200 years ago) and ^{137}Cs (from bomb tests) in relation to sediments. The existence of input and validation data is an important criterion in the choice of constituents modelled.

The whole exercise is in effect a sensitivity analysis.

2.4 Ecosystem models.

Two can presently be envisaged: offshore in the water column; salt marsh.

The ERSEM model has already been applied to ten regions of the North Sea, simulating the seasonal cycles of all major pelagic and benthic groups and their interactions with nutrient status. It runs under SESAME, includes hydrodynamics from IfM Hamburg aggregated to

ICES boxes, can accommodate other modules and is envisaged as the basis for a coastal carbon model, but is concerned strictly with areas covered by sea. ERSEM will be available for general use in mid-1993.

Validation. Comparison with RACS measurements of N, P, Si, chlorophyll, O_2 implicated in the carbon cycle.

Strictly coastal ecosystems (notably saltmarsh, for which there are several RACS expressions of interest) should be addressed later in LOIS according to activity in other components that are conceptually "upstream". (Other contacts: SOAFD, Prof W Gurney - Strathclyde, PML, UCNW, Wood - Silwood Park, Ollason - Aberdeen, Ann Jones - Paisley, Warren - Sheffield). There is as yet no expression of interest for prognostic modelling.

2.5 Shelf evolution

Runs of the shelf-wide wave/tide/surge model as in 2.2 *geomorphology* with the addition of sediment transport, again for "time-slices" with past scenarios, then speeded-up bed evolution in response thereto (eg. Belfast & POL, UCNW, BGS & Durham). The contribution from deposition of plankton detritus etc. may be important locally and needs initial assessment shelf-wide.

Validation. Required data should be available from Durham, BGS *via* LOEPS.

2.6 Shelf-sea budgets

Model as in 2.1 *Water Quality.* Model equations imply closed budgets on the model grid scale; wider budgets will be estimated by integration of fluxes through time across sections aggregating grid-box boundaries. This study emphasises the modelling of Fe, Al and/or Mn.

2.7 Management tools

To be discussed with potential commissioning authorities.

2.8 System

For all objectives, which are not operational in a real-time sense for LOIS, the need for two-way exchange is infrequent enough to allow any atmospheric, catchment and oceanic (input) model to be run first offline. The *catchment*-estuary model boundary should be upstream of any turbidity maximum, natural boundary (freshwater interface) or tidal effect on fluxes along the river (avoiding any need for feedback to the catchment model apart from a possible ponding effect); the most downstream river-gauging station might be a suitable pragmatic choice of boundary; the estuary model should extend upstream to this point. At the *ocean* boundary, it is familiar and reasonable to specify the ocean tide, and reasonable to specify an observed rather than an on-line model value for oceanic nutrients, for example. The treatment of phenomena such as upwelling, and their effect on shelf circulation, is less clear. SES would only study a small sector of shelf edge, but any model must include a large area to the south, most probably through embedding in the shelf-wide NORMS model. There is an objective to couple the shelf-wide water quality model to an oceanic model (eg. OCCAM or ...) by 1997.

A modular framework will be used with a common grid, for all interactive variables. POL report # 19 (J. Wolf) provides a prototype. In cases such as waves where the use of a fine grid would entail excessive computation, an interpolating shell to the module will be used, so that the grid appears to be common. The framework will define interfaces to facilitate parallel development and substitution of programmes (modules) for individual constituents and processes, while realising the integration of different disciplines for the above objectives. Offline data transfers will require (later) agreement on grids and formats taking account of data exchange protocols elsewhere.

NORMS models are expected to be run by relatively few and experienced modellers; a user-friendly shell (such as the menu-driven interface which drives ECoS) or expert system front end would be a priority only for commissioned funding later in relation to model use for management or policy. However, programmes should be in *FORTRAN* or *C* language, a compromise between compatibility (routines in each can be called by a programme in the other) and respect for "investment" in both languages hitherto.

2.9 Data

Data input to models, sharper model-data comparison, and hence related interpolation, appear to be the main NORMS modelling interests in GIS-type techniques, with expert systems as a development appropriate for departmental funding. Extension from data input to assimilation and initialisation of models is a technical model-dependent question involving the modeller's specialist expertise. For model validation, it may be appropriate to "fly the instrument through the model". Alternatively, GIS techniques could provide a link between CASI data and a phytoplankton model (say). Interpolations for comparisons should include error estimates.

3. Resources

Large requirements are a fast processor, and networking (super-JANET). Of smaller cost but wide interest through LOIS, are workstations (with common operating systems, possibly the subject of a bulk purchase), a visualisation "package" for data and model output.

3.1 Finances (£K) (to be re-formatted when skeleton is available from LOIS management)

costs	1992/93	1993/94	1994/95	1995/96	1996/97
a) salaries	+	80+	100+	100+	80+
b) equipment (<£30K)		40	+	+	+
c) T&S (workshops)	1	2	2	2	2
d) overhead (0.4 a)		32+	40+	40+	32+
e) large capital	700				
f) data					
g) NCS superstruct?					
financed by					
LOIS responsive	50	80	140	130	130
specific capital	700				
institute baseline	+	+	+	+	+

(2 at POL, divided between baseline and DoE + EC commissions)

commissions (DoE, MoD, EC, NRA, MAFF - fisheries and flood defence)

There is NRA interest in: source-sink water-quality modelling in estuaries and nearshore; proportional "damage" to the North Sea by individual rivers (relates to *water quality* objective); ability to estimate effects of policy options - consents, sludge dumping etc. by the UK and possibly others: all these more as long-term effects than hour-by-hour.

4. Timetable

1992 | 1993 | 1994 | 1995 | 1996 | 1997

<u>water quality</u>
hydrodynamics
3-D 20km given T,S
3-D, 3 km, Dover Strait-56°N evolving T,S - extend shelf-wide
1 km shelf edge - develop - nest into shelf-wide
suspended sediment, phytoplankton - 1-D with hydrodyn. - nearshore 3-D - into shelf-wide
nutrients, metals, oxygen - 2-D - develop sources, sinks - into 3-D - shelf-wide
---- compare with constituent distributions ----

<u>coastal geomorphology</u> (shelf evolution similar)
nearshore wave model development
coastal strip model - develop - add waves - empirical - with waves driving sediment
catchment/river model - develop - scenarios
shelf model - waves interaction - scenarios
LOEPS cores - collection - analysis - input - as test data

<u>buffering</u>
coastal strip model - develop - especially sediment transport - combined scenarios
catchment/river model - develop - scenarios
shelf model - scenarios
RACS/LOEPS data - collection - analysis - input - as test data (comparison)

5. Relation to other LOIS components

NORMS will provide a synthesis of other LOIS components in the following respects. The shelf-wide (water-quality) model of NORMS will include detailed models of the RACS coastal and SES areas, and link their transports or fluxes in an implicit shelf-wide budget. The *buffering* and *geomorphology* studies link RACS river and coastal components into the wider spatial and temporal perspective of LOEPS.

There are needs of data from other LOIS components: water-quality constituents from RACS, physics and biogeochemical processes from RACS coastal and SES, cores and crustal model results from LOEPS.

APPENDIX 3

WRSRU Subsurface Flow and Transport Model

A computer based numerical modelling system capable of simulating flow and transport processes in complex geological environments for one- two- or three-dimensional problems is under development by staff of the Water Resource Systems Research Unit. The first phase of development of this modelling system is due for completion in December, 1993. It is being developed as a 'state of the art' modelling package capable of working over a wide range of spatial and temporal scales and for a wide range of pollutants as well as in diverse geological environments.

The modelling system comprises three component models designed for specific problem areas that are integrated together through a single management shell. The three components comprise (i) a one dimensional unsaturated/saturated zone model for multi-component, multi-species transport, (ii) a quasi three dimensional model for regional groundwater flow and transport and (iii) a three dimensional model for detailed analysis of groundwater flow and transport involving complex natural and engineered hydrogeological systems.

To indicate the capabilities of the modelling system for simulating flow and transport phenomena the following summary description of the three dimensional component is reproduced:

Conceptual Framework:

1. Only flow and transport in groundwater is modelled.

2. The upper boundary of the model is defined by the position of the phreatic surface of the upper aquifer (unconfined) or the top of the upper aquifer (confined)

3. The lower boundary of the model is defined by the base of the lowest geological unit apparently contributing to substantial groundwater flow.

4. Flow and transport are three dimensional.

5. Flow and transport may occur within a formation in any one of three zones of a

geological unit. These zones comprise - solution enlarged fissure pathways or channels; permeable strata or finely spaced joint systems and, finally, low permeability strata with significant porosity. The nature of the zones and their connectivity is dependent on the nature of the formation to be represented.

6. Distinct hydraulic models are to be used to describe flow and transport in the engineered region of wells or adits or in the vicinity of surface flow systems whether terrestrial or marine.

7. Each formation may be modelled using heterogeneous, anisotropic rock property distributions.

8. Internal processes that are being represented in the model comprise:

Single phase flow and transport only;
Density dependent Darcian flow for low Reynolds number environments, non-Darcian flow processes for high Reynolds number environments.
Chemical and Biodegradation reactions for up to three coupled chemical species.
Non-linear and linear adsorption in each zone of the formations.
Time independent rock properties.
Time independent temperature distributions.

Numerical Framework

A ' Finite Volume' numerical scheme has been employed for the solution of the groundwater flow and dispersion equations. A deformable quadrilateral mesh permits grid refinement for regions of interest. Geological formation structures can be matched readily using this type of grid. The grid is efficiently constructed using an interactive package. A multi-grid matrix solver is used to solve the set of linearised equations.

A moving point method is implemented for the solution of the transport equations. The flow and transport solutions may be uncoupled, loosely coupled or fully coupled depending on the accuracy of the solution required.

The model is to be mounted on a fast workstation and will be capable of working with meshes exceeding 10,000 nodes.

The 3D model is in part based on an existing code developed within the WRSRU for the simulation of flow in large multi-aquifer systems - FDMOD. FDMOD has been recently used to study the flow characteristics of the aquifers in the area around Harwell as part of a study of the impact of the hypothetical disposal of toxic waste in the Oxford Clay. The model simulated flows over an area of 40km x 50km and incorporated descriptions of the 10 major geological formations found in the vicinity of the site. A 25,000 node mesh was used and the simulations performed on a SUN Sparc 1 workstation.

RM 29/9/92.

APPENDIX 4

The Nitrogen Model Mass Balance Equation

NITROGEN BALANCE PROCESSES

External sources

1. **Wet and dry atmospheric deposition**
   Estimated from published national figures.

2. **Fertilizer and manure application**
   Obtained from agricultural records.

Internal transfer

Transformation

Transformations described here are those used in the SOILN and LEACHN models. The reactions given are those for a particular soil layer.

1. **Mineralization of humus**

$$N_{h \to NH_4} = k_n e_t e_m N_h$$

k_n : specific mineralization constant, e_t : soil temperature factor, e_m : soil moisture factor and N_h : N–content in humus.

2. **Net mineralization or immobilization of N in litter**

$$N_{l \to NH_4} = [N_l/C_l - f_e/r_0] C_{l(d)}$$

f_e/r_0 : equilibrium C–Nratio, C_l soil litter carbon, $C_{l(d)}$: decomposed soil litter carbon.

3. **Nitrification of ammonium to nitrate**

$$N_{NH_4 \to NO_3} = k_n e_t e_m [N_{NH_4} - N_{NO_3}/n_q]$$

k_n : potential nitrification rate and n_q : nitrate–ammonium ratio

4. **Plant uptake of nitrogen**
   The uptake of nitrogen is computed as the function U(t) where:

$$\int_{t_0}^{t} U(\tau) d\tau = U_a / [1 + ((U_a - U_b)/U_b) e^{-U_c (t - t_0)}]$$

U_a : potential annual N uptake, U_b and U_c : shape parameters and t : days after the start of the growing season, t_0.

Transport

Homogeneous porous medium

1. **Convection dispersion**

   A single equation may be applied for homogeneous soils. For vertical flow this may be written:

   $$\partial \theta c / \partial t = -\partial / \partial z[-(\theta D_m(q) + D_p(\theta)) \partial c / \partial z + qc]$$

   θ : volumetric water content, c : solute concentration, t : time, z : depth, D_m : mechanical dispersion coefficient, q : volumetric water flux and D_p : effective diffusion coefficient.

Inhomogeneous porous medium

1. **Convection dispersion**

   A modified equation may be used for soils with mobile and immobile water:

   $$\partial \theta_m c_m / \partial t = \partial / \partial z[D_m \theta_m \partial c_m / \partial z] - q \partial c_m / \partial z - \alpha \theta_m (c_m - c_{im})$$

   $$\partial \theta_{im} c_{im} / \partial t = \alpha \theta_m (c_m - c_{im})$$

   θ_m : water content in the mobile water phase, θ_{im} : water content in the immobile water phase, c_m : concentration in the mobile water phase, α : mass transfer coefficient and c_{im} : concentration in the immobile water.

Sinks

1. **Denitrification**

   This is as described in SOILN and LEACHN for a particular soil depth:

   $$N_{NO_3} = k_d e_{md} e_t \{N_{NO_3} / (N_{NO_3} + C_s)\}$$

   where

   $$e_{md} = [(\theta - \theta_d)/(\theta_s - \theta_d)]^d$$

   θ : soil water content, θ_s : soil water content at saturation, θ_d : a threshold point, d : empirical constant, N_{NO3} : denitrification rate, k_d : potential denitrification rate and C_s : half-saturation constant.

3. **Harvest**

   Removal of organic N in the harvested crop is estimated from measured yield crop. Material remaining in the field enters the organic nitrogen pool.

ADDITIONAL PROCESSES

The water and nitrogen cycles are influenced by driving variables other than water and N inputs.

The water balance is greatly influenced by temperature through its effect on evapotranspiration. This is accounted for in the expression for evapotranspiration, and values are obtained from meteorological field data.

The N cycle is also influenced by temperature in the soil, which is not available but must be estimated from surface and soil conditions. The nitrogen cycle is also intimately bound up with the carbon cycle, the C/N ratio determining whether immobilisation or mineralisation is dominant. The carbon cycle is incompletely considered in this modelling. A fuller treatment would include C as a state variable.

The water and N balance processes described are those which are likely to be important at Brimstone. Others such as ammonia volatilisation and biological N fixation may need to be included at different sites.

APPENDIX 5

Water Res. Vol. 18, No. 8, pp. 945–953, 1984
Printed in Great Britain.

0043-1354/84 $3.00 + 0.00

MODELLING ALGAL BEHAVIOUR IN THE RIVER THAMES

P. G. WHITEHEAD[1] and G. M. HORNBERGER[2]

[1]Institute of Hydrology, Wallingford, England and [2]Department of Environmental Sciences, University of Virginia, Charlottesville, VA 22903, U.S.A.

(Received August 1982)

Abstract—Forecasting the movement and growth of algae in river systems is particularly important for operational managers responsible for the distribution and supply of potable water. Algae affect the taste and smell of water and pose considerable filtration problems at water treatment plants. In a collaborative study with the Thames Water Authority, algal models have been developed for the River Thames. The non-linear processes controlling algal growth are examined using a generalized sensitivity analysis technique and the dominant parameters controlling system behaviour are identified. The extended Kalman filter (EKF) is then used to estimate these important parameters. The technique of using generalized sensitivity analysis prior to EKF estimation is suggested as a pragmatic approach to the problem of identifying the subset of physically, chemically or biologically meaningful parameters controlling system behaviour in mechanistic models.

Key words—algal models, River Thames, model identification, parameter estimation, sensitivity analysis, Kalman filter, water quality modelling

INTRODUCTION

With the increasing demands on the Thames as the principal source of water for London, it is not surprising that in recent years concern over present and future water quality has been expressed. Water quality problems of immediate interest to the Thames Water Authority reflect the multiple use of the river as the principal disposal pathway of industrial and domestic effluent in addition to being a major source of water for agricultural, industrial and domestic purposes. In particular, progressively increasing levels of nitrates in surface and groundwater systems have exceeded WHO and EEC standards and the Thames Water Authority have restricted abstractions during periods when concentrations of nitrate in the river are high (Onstad and Blake, 1980). Furthermore, major algal blooms occur on the river and these present operational management problems for the Water Authority. Abstracted water is pumped into reservoir storage prior to distribution to water treatment plants and algal growth affects water taste and smell and causes filtration problems. The prediction of algal growth, transport and decay is, therefore, of considerable importance in water supply management. In the paper an algal model is described and a sensitivity analysis technique utilized to identify key parameters controlling algal behaviour. Finally, the extended Kalman filter is employed to estimate these parameters using data from the River Thames.

MODELLING APPROACH

Mass-balance model

Algal distribution and growth processes in the River Thames have been the subject of research by a number of biologists this century (Fritsch, 1902, 1903, 1905; Rice, 1938; Kowalczewski and Lack, 1971; Lack, 1971; Bowles, 1978), but modelling techniques have not been used heretofore to obtain an adequate description of the system. There have been few modelling studies of algal growth and transport processes in rivers in general, although the analysis of flow and quality data using modelling techniques have developed considerably in recent years (Thomann, 1972; Beck and Young, 1976; Whitehead *et al.*, 1979, 1981). In this paper the development of mechanistic models for algal transport and growth is stressed. By mechanistic we mean a model containing mathematical expressions for the various physical, chemical and biological phenomena controlling system behaviour. We examined initially a mass-balance model as applied to three years of weekly algal data over 1974, 1975 and 1976 for six reaches of the river shown in Fig. 1.

The aim of this study was to determine to what extent transport alone could explain the observed variations in chlorphyll-*a* data. The results of this analysis are given in Whitehead and Hornberger (1984). It was found, not surprisingly, that transport alone could not account for the observed variations in algal levels but that complex processes of algal growth and death or sedimentation were occurring. In order to model such behaviour it is necessary to hypothesize mechanisms for these processes.

Rather than take a standard model developed for a particular system the approach herein has been to evaluate the most likely factors controlling algal growth and losses and to represent these mathe-

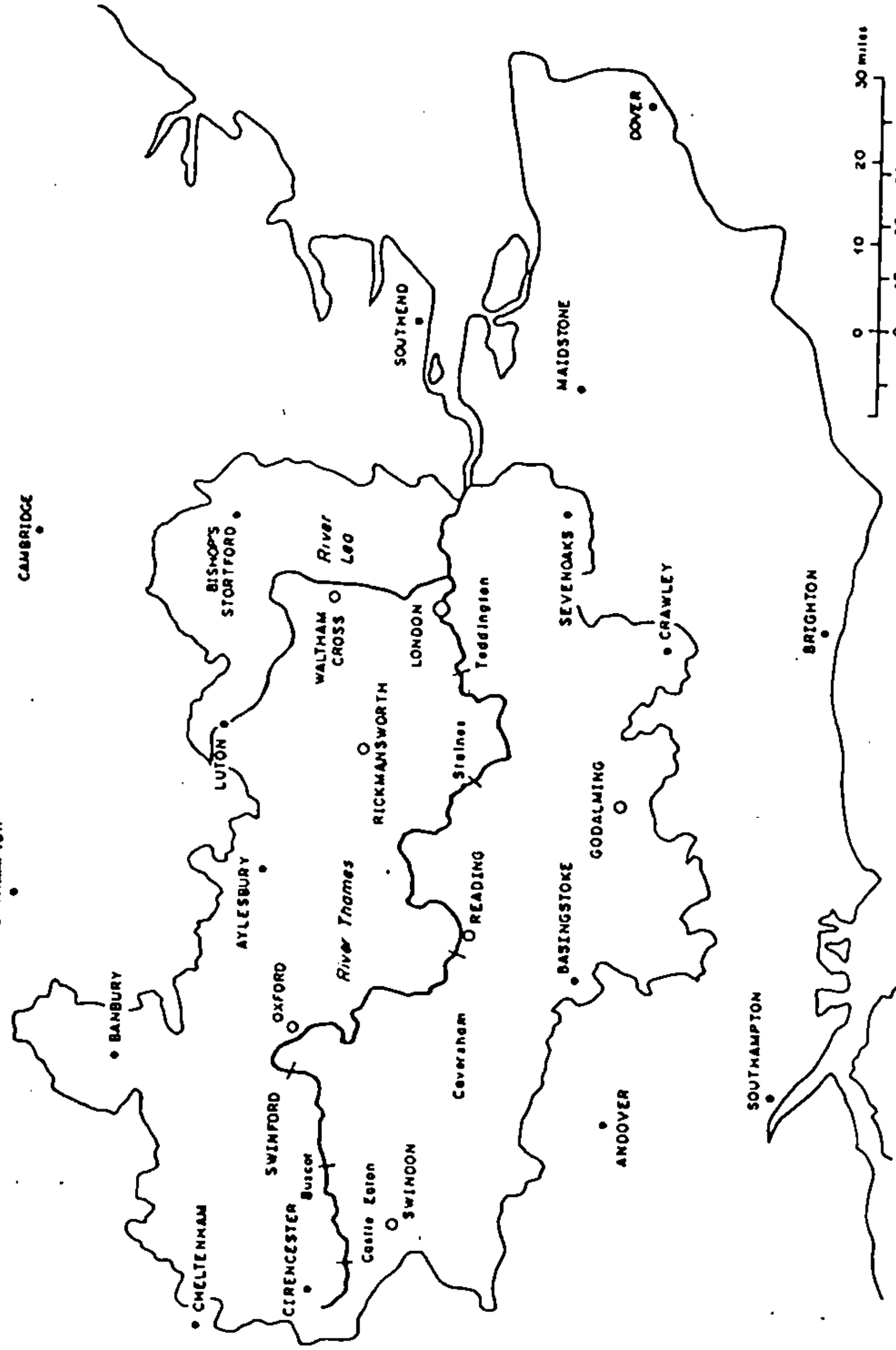


Fig. 1. The Thames catchment area (reach boundaries at Castle Eaton, Buscot, Swinford, Caversham, Staines and Teddington).

matically. The four factors considered particularly important for algal growth are:

(i) the growth coefficient;

(ii) the effect of solar radiation which under conditions of unlimited nutrient availability provides the main driving force for algal growth;

(iii) the effect of turbulence which tends to increase with increasing flow causing resuspension of sedimented material and reducing light penetration;

(iv) the self-shading factor in which algal populations grow to the point where light penetration is reduced by algae themselves.

The loss processes were assumed to be related to the concentration of algae via a first order decay term but nonlinear forms were used for the light limitation terms. The basic mass balance equations for describing concentrations of live and dead algae are similar to those developed by Beck (1978) but include mathematical terms to describe the four factors discussed above. The equations are as follows:

Live algae

$$\frac{dx_1(t)}{dt} = k_1 Q_i(t)\,u(t) - k_1 Q_o(t)\,x(t) - k_2 x_1(t) + k_3 \frac{I(t)}{Q_o(t)} \left(\frac{k_4}{k_4 + (x_1(t))^{k_5}}\right)\left(\frac{I(t)}{k_6}\right)^{k_7} \times \exp\left[1 - \left(\frac{I(t)}{k_6}\right)^{k_7}\right]. \qquad (1)$$

Dead algae

$$\frac{dx_2(t)}{dt} = -k_1 Q_o(t)\,x_2(t) + k_2 x_1(t) - k_8 x_2(t) \qquad (2)$$

where $x_1(t)$ and $x_2(t)$ represent the live and dead algae respectively at the output (downstream) boundary of the reach, measured as chlorophyll-*a* ($\mu g\ l^{-1}$); $u_1(t)$ represents the input (upstream) algae concentration ($\mu g\ l^{-1}$); $Q_i(t)$ and $Q_o(t)$ represent the upstream and downstream flow rates; $I(t)$ is the solar radiation level ($W\ cm^{-2}$); k_1 determines the residence time characteristics of the model such that $k_1 Q_o(t) = 1/\tau$ where τ is the residence time; k_2 is the algal death rate; k_3 is the growth coefficient; k_4 is a half-saturation level for the self-shading function. $\{k_4/[k_4 + (x_1(t))^{k_5}]\}$ and k_5 is included as a power term on $x_1(t)$ to enhance the self-shading factor at high algal concentrations; k_6 represents the optimal solar radiation level in the term $[I(t)/k_6]^{k_7} \exp\{1 - [I(t)/k_6]^{k_7}\}$ which accounts for the decrease in algal growth under low light intensity and the apparent decrease in growth under extremely high light intensity conditions in the Thames (Steele, 1978); k_7 enhances the effect of this solar radiation term; k_8 is included in the dead algae equation to account for the loss of algae by sedimentation. An additional parameter k_9 is included in the model as a temperature threshold below which algal growth is zero, i.e. $k_3 = 0$ for $T < k_9$ where T is water temperature °C.

Estimation of model parameters

Many researchers have developed phytoplankton growth models for simulation purposes. In general, the approach to parameter estimation has been to select parameters quoted in the literature and assume that these values pertain to the system under investigation. Formal methods of parameter estimation have been used in few studies; e.g. Lederman *et al.* (1976) applied non-linear parameter estimation techniques to data from batch cultures of phytoplankton to directly estimate model parameters and Whitehead (1980) used an instrumental variable algorithm applied to differential equation models of water quality to estimate parameters. In this paper the extended Kalman filter (EKF) technique has been used to estimate model parameters.

The EKF is a recursive algorithm in which an estimate of the unknown parameter vector $\hat{a}$ is updated while working serially through the data. The estimate $\hat{a}$ of a at the kth instant in time is given by an algorithm of the following form:

$$\hat{a}_k = \hat{a}_{k-1} + G_{k|k-1}\{y_k - \hat{y}_{k|k-1}\} \qquad (3)$$

where the second term on the right hand side is a correction factor based on the difference between the latest measurement y_k and the estimate $\hat{y}_{k|k-1}$ of that determinand derived from the model using estimated model coefficients obtained at the previous time point. $G_{k|k-1}$ is a weighting matrix whose elements are calculated essentially as a function of the levels of uncertainty (or error) specified for the model in the output response and the unmeasured input disturbances. A full description of the technique can be found in Jazwinski (1970) or Young (1974) and applications of the EKF for modelling nitrate, chloride, dissolved oxygen and BOD are given by Whitehead *et al.* (1981) for the Bedford Ouse River system and by Beck and Young (1976) for the River Cam.

Estimating parameters in mechanistic models is often difficult because of the non-linear nature of the process equations and the interdependence of parameters. In the case of the algal model there are nine interrelated parameters to determine and estimation is particularly difficult. This is an important aspect of the modelling study since it is generally not possible to obtain reliable estimates of the large number of parameters in most simulation models. It is preferable to eliminate parameters that cannot be identified with a given data set or to set those parameters which are thought to be well known and to then estimate the remaining parameters. Up to now there has been no systematic method of selecting the subset of parameters for optimization. A trial and error procedure is normally used to select these parameters but given the non-linear nature of most simulation models such an approach can present problems of interpretation and is certainly not rigorous. A generalized sensitivity analysis can aid in this parameter selection to ensure that the optimal set of parameters are obtained. Such a technique has been developed by Spear and Hornberger (1980) and applied to aquatic ecosystem problems by Hornberger and Spear (1981).

Generalized sensitivity analysis

The generalized sensitivity analysis technique is based on the utilization of a simulation model together with a classification algorithm. The classification algorithm allows the model outputs to be identified as either representative or as not representative of the observed behaviour. The idea is to inject uncertainty into the simulation model by selecting the parameters from specified probability distributions rather than from experimentally derived values. The simulation is repeated using different parameter sets and the parameter set classified as either producing or not producing a behaviour. Subsequent to these Monte Carlo trials, statistical analysis of the parameter sets is used to identify the key parameters causing the model to reproduce the observed behaviour. The theory behind this statistical analysis is based on the separation between the cumulative probability distributions of two parameter sets, and a Kolmogorov–Smirnov two sample test is utilized to test the separation. The test is described by Spear and Hornberger (1980) and the statistic $d_{m,n}$ is determined as the maximum vertical distance between the cumulative probability distribution curves for n behaviours and m non-behaviours. Thus, large values of $d_{m,n}$ indicate that the parameter is important for simulating the behaviour. The value of $d_{m,n}$ can be compared with a 90% confidence bound value to check that it is statistically significant. Further refinements of the technique are presented by Spear and Hornberger (1980) and Hornberger and Spear (1980, 1981).

APPLICATION TO THE THAMES ALGAL MODEL

In the algal modelling study on the Thames it is first necessary to define the system behaviour. The two important features of algal growth within the river are the presence of a spring bloom and the subsequent fall to relatively low levels in early summer. On this basis simulations are classified as a behaviour if the algal concentration, x_1, is at any time, above 100 $\mu g\ l^{-1}$ and below 400 $\mu g\ l^{-1}$ during a 5 week period in spring and if, in addition x_1 falls below 100 $\mu g\ l^{-1}$ and remains below this level for at least 2 weeks during the 5 weeks after the spring bloom.

The model parameters were selected initially on the basis of published information such as travel times for the Thames determined by the Water Authority or growth rates for algae in the Thames. As previously discussed there is considerable uncertainty associated with many of the parameters in the model. In the case of growth rates, for example, Swale (1962), measured a growth rate for *Stephanodiscus hantzschii* of 0.46 day^{-1} and Bowles (1978) determined a growth rate for *Asterionella* of 1.28 day^{-1} from loading studies on the Thames. Lund (1949) also determined a growth rate for *Asterionella formosa* of 1.73 day^{-1} under ideal growth conditions although this reduced to 0.138 day^{-1} under field conditions. The situation in the Thames is complicated by the changing nature of the river with relatively slow flow in the lower reaches compared with the flow in upper reaches between Buscot and Swinford.

A complete list of the mean parameter values for the Monte Carlo simulation runs is given in Table 1. In the Monte Carlo runs the parameter values are

Table 1. Monte Carlo simulation results for reach 5 of the River Thames

Monte Carlo simulation runs	1		2		3		4
Critical $d_{m,n}$ at 90% confidence level	0.326		0.430		0.470		*
Parameter value (P) Distribution separation (S)	P	S	P	S	P	S	P
k_1 related to travel time τ, $k_1 Q_a = 1/\tau$	0.5	0.2	0.16	0.14	0.16	0.34	0.16
k_2 algal death rate (weeks^{-1})	0.3	0.2	0.3	0.16	0.3	0.19	0.6
k_3 algal growth rate (weeks^{-1})	10	0.15	8.0	0.33	10	<u>0.48</u>	12
k_4 algal saturation level ($\mu g\ l^{-1}$)	100	0.17	100	0.1	100	0.17	100
k_5 power in saturation term	2	<u>0.73</u>	2.5	<u>0.68</u>	3	<u>0.87</u>	4
k_6 optimal solar radiation (W hours cm^{-2} per week)	20,000	<u>0.51</u>	13,000	<u>0.5</u>	15,000	<u>0.51</u>	10,000
k_7 power in light attenuation term	2	0.30	2	0.42	2	0.31	2
k_8 sedimentation rate (weeks^{-1})	0.3	0.13	0.3	0.26	0.3	0.25	0.3
k_9 temperature threshold effect (°C)	8	0.11	8	0.16	8	0.17	8
% behaviour (based on 100 simulations)	48%		79%		86%		98%

*Statistics invalid since distribution of non-behaviours indeterminable from 2% of simulations

Table 2. Statistics for 9 parameters in simulation run 1

Parameter	Normalized mean under behaviour	Normalized mean under non-behaviour
k_1	0.21	−0.10
k_2	−0.24	0.57
k_3	−0.10	0.18
k_4	0.62	0.21
k_5	0.54	−0.70
k_6	−0.56	0.42
k_7	0.34	−0.24
k_8	−0.84	0.53
k_9	−0.11	−0.18

selected randomly assuming a rectangular distribution with a range of ±50% of the mean of the parameter. This ensures that a wide spread of parameter values is selected and that behavioural patterns are fully explored.

Table 1 shows the parameter values used in four sets of Monte Carlo simulations together with the maximum separation between the parameter distributions and the critical separation $d_{m,n}$ at the 90% confidence level. It is particularly interesting to note that relatively few parameters appear to be significant in determining behaviour. Over the four simulations only three parameters are clearly identified as critical, these being the growth rate k_3, the power term in the saturation factor k_5 and the optimal solar radiation level k_6. In the first simulation only 48% of the runs satisfy the behaviour criteria. From analysing the behaviour-producing parameters it is possible to determine whether to increase or decrease the mean values of parameters in order to increase the percentage of behaviour. For example, in the case of the power term parameter k_5 in the saturation function, the normalized mean under the behaviour is 0.54 as shown in Table 2 suggesting that this parameter should be increased. By increasing this parameter the shape of the saturation function is altered thus enhancing the effect of the saturation level. Similarly in the case of k_6, the optimal solar radiation level, the normalized mean is −0.56 suggesting a reduction in this parameter. The Monte Carlo simulations therefore can be used as a crude estimation procedure and the percentage of behaviours increased from 48 to 98% over the four runs using this approach.

From a systems point of view what is particularly significant is that only three of the nine parameters control system behaviour. In most modelling studies of ecological or hydrological systems it is conventional to assume that each parameter is equally important. As previously mentioned, in many simulation studies a trial and error procedure of model calibration occurs in which a subset of the parameters is adjusted until a reasonable model fit is obtained. With large complex models this process can be particularly difficult because of interactions between parameters and mechanisms. The generalized sensitivity analysis approach can therefore be used in this situation to determine the dominant parameters controlling behaviour in a systematic manner.

APPLICATION OF THE EKF

In the Thames algal model is proved impossible to apply a technique such as the extended Kalman filter to estimate all nine parameters. The EKF technique applied in this situation gives parameter values which are either clearly incorrect or show colinearity in which one parameter increases as another decreases to cancel out its effect. Thus in order to obtain reasonable parameter estimates the EKF is applied to the three critical parameters indicated by the sensitivity analysis with the remaining parameters set to values estimated from independent laboratory or field measurements.

The estimation results obtained by the EKF for the fourth and fifth reaches are typical of those for the

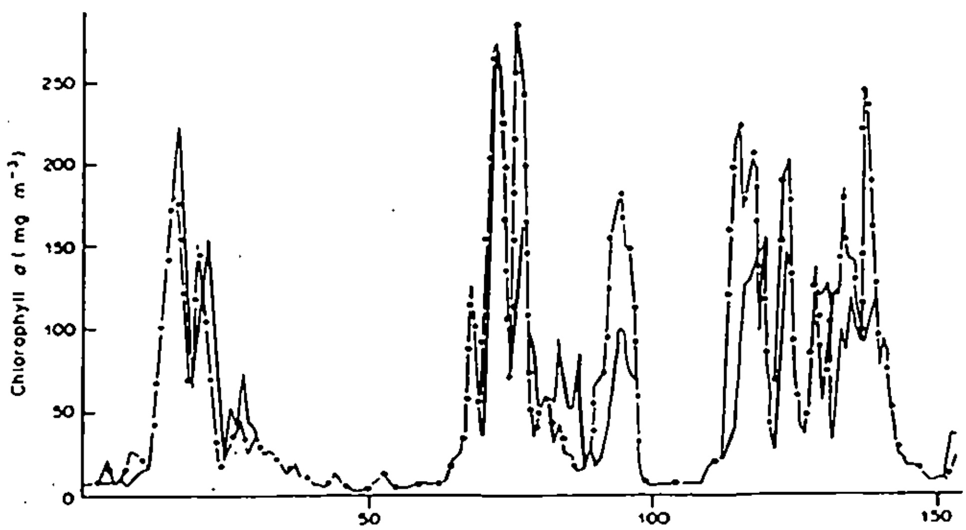


Fig. 2. Estimated (——) and observed (●) chlorophyll-a for 5th reach.

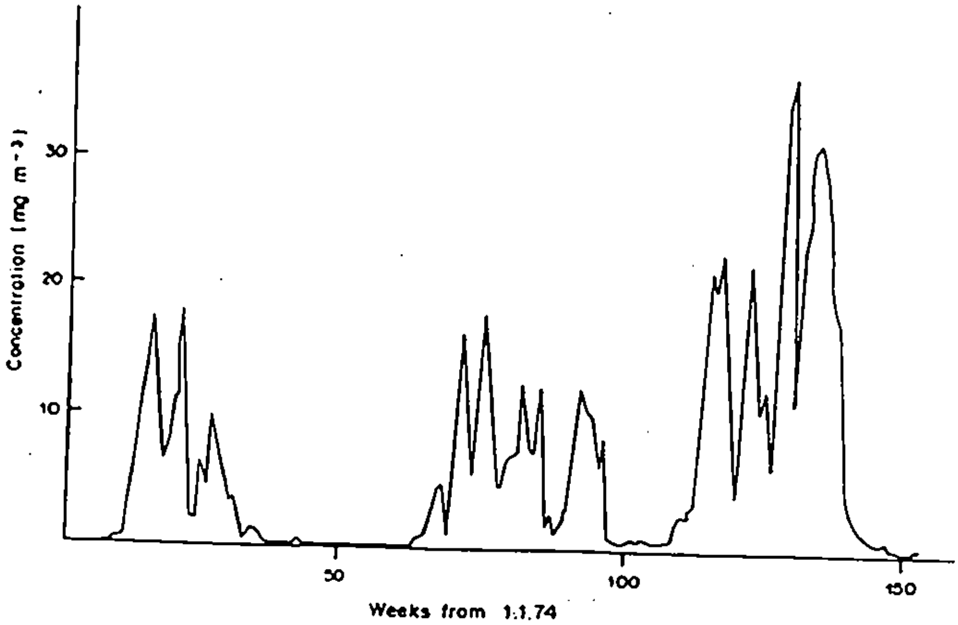


Fig. 3. Estimated state x_2 (dead algae) in 5th reach.

entire stretch of river considered. Figures 2, 3 and 4 for the fifth reach show, respectively, the estimated and observed chlorophyll-*a*, x_1, the estimated "dead" algal state, x_2, and the parameter estimates obtained from the EKF analysis. In general, the estimated values correspond well with the observed chlorophyll-*a* values and the parameters k_3, k_5 and k_6 are reasonably time invariant. The parameters show some movement at week 90. This corresponds with a data period when the model estimate is below the observed levels; in this situation the parameters are adjusted by the EKF algorithm to compensate for the lack of fit. Figure 5 shows the pheopigment levels for the same simulation time period. Comparing Figs 3 and 5 one observes that the dead algal estimate, x_2, compares reasonably with the observed pheopigment levels. The pattern of behaviour and concentration levels are similar and it appears possible to use the pheopigment as a surrogate measure of dead algae within the reach.

The simulation results and parameters obtained by the EKF analysis for the fourth reach, as shown in Figs 6 and 7, are more variable than those for the fifth reach. The power in the algal saturation term reduces from 4 down to 3.3 and the growth coefficient increases over the 1976 summer period. These changes may be due to the different types of algae dominating the river system. For example in summer 1976 there was a major bloom of *Microcystis* and self-shading is different because of the different size,

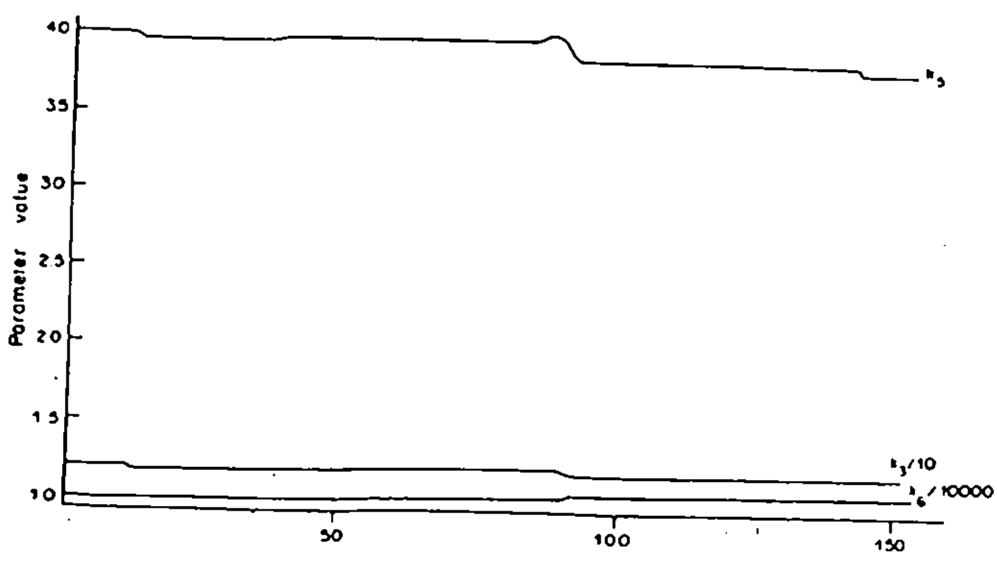


Fig. 4. Estimated model parameters k_3, k_5 and k_6 for 5th reach.

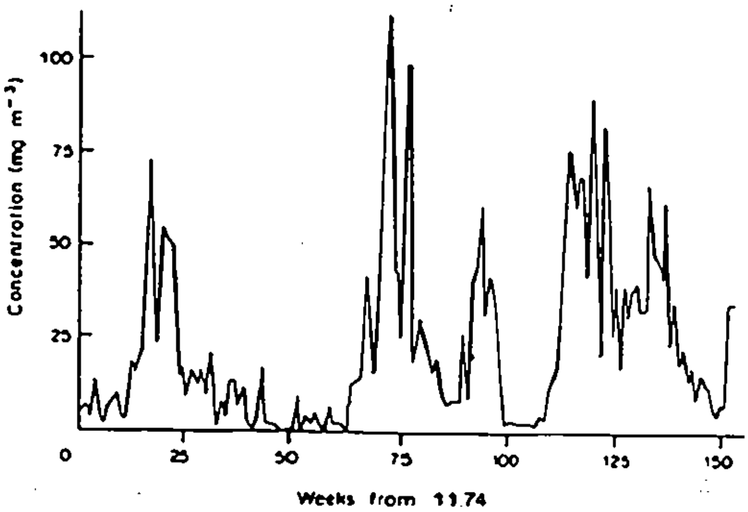


Fig. 5. Pheopigment concentrations in River Thames over 1974, 1975 and 1976.

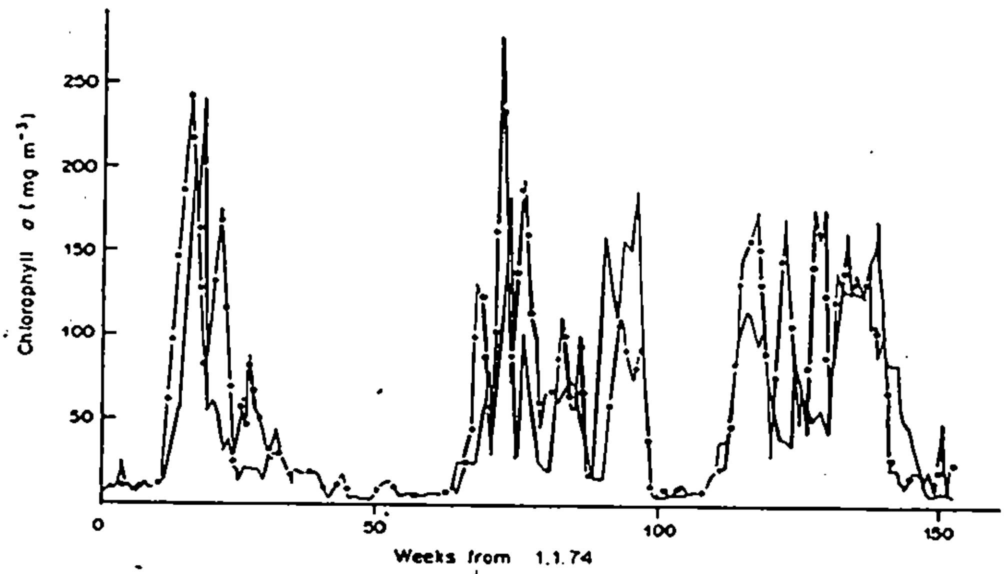


Fig. 6. Estimated (——) and observed (●) chlorophyll-a levels in 4th reach.

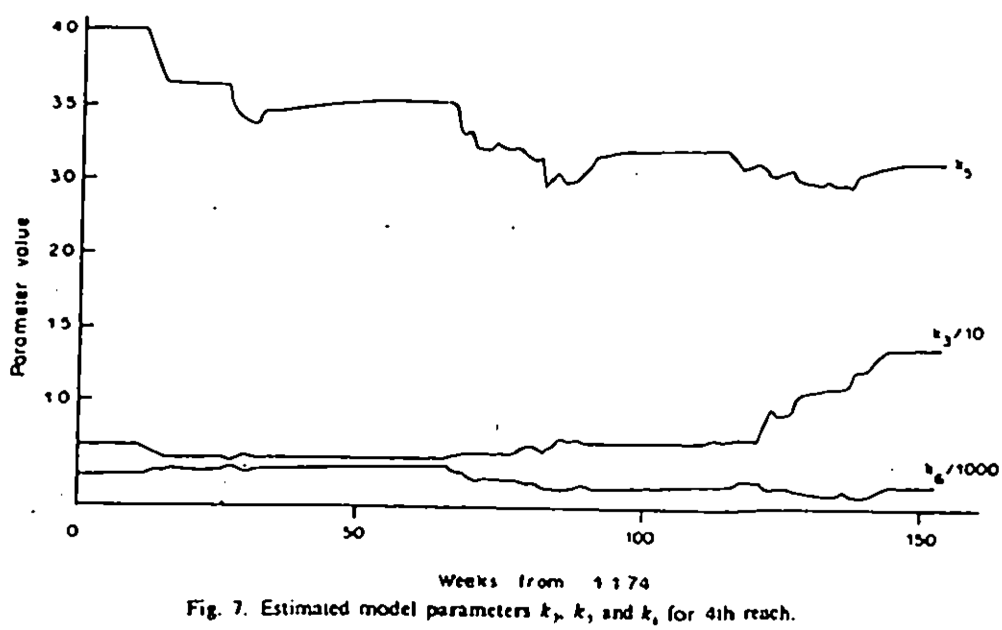


Fig. 7. Estimated model parameters k_3, k_5 and k_6 for 4th reach.

clustering and buoyancy characteristics of *Microcystis* compared with other algae. Thus, although the time variation of parameters in reach 4 is greater than for reach 5, the variation is not extreme and corresponds to observed biological changes in the river.

APPLICATIONS OF THE ALGAL MODEL

The algal modelling study has been undertaken within the context of an extensive Thames nitrate modelling project (Whitehead and Williams, 1982). Having established a satisfactory model for forecasting algal (chlorophyll-*a*) concentrations, it is possible to consider combining the algal and nitrate model to account for the uptake of nitrate by growing algae and subsequent recycling of nitrate after algal death. At present, the nitrate model simulates the overall loss processes which include denitrification and algal uptake by a single temperature dependent first order rate coefficient (Toms *et al.*, 1975). Linking the algal model to the nitrate model would provide a means of separating these processes thereby improving the predictive capability of the model.

A second area of application is the forecasting of algal levels at key abstraction sites along the Thames. A daily version of the model could be used in a real time context to provide operational management with estimates of day to day concentrations. A similar on-line scheme for operational management has already been established on the Bedford Ouse to forecast such variables as nitrate, dissolved oxygen and ammonia (Whitehead *et al.*, 1983). In this case, data from water quality outstations are telemetered to a control mini-computer and forecasts of flow and quality are obtained using a mathematical model stored in the computer. A similar scheme could be established on the River Thames to provide information to water resource managers on the movement of algal blooms down the river.

CONCLUSIONS

The complex dynamic behaviour of algae within river systems has been studied using a number of systems analysis techniques. Where algal growth processes dominate, a mechanistic model is required to account for the highly non-linear behaviour. In this situation model identification and estimation is particularly difficult and a generalized sensitivity analysis technique can be used to determine the important parameters and hence restrict the number of parameters requiring estimation.

In the case of the Thames algal model three significant parameters have been identified out of the nine model parameters using the generalized sensitivity analysis technique. Having identified these parameters the EKF technique has been applied to estimate final parameter values.

The application of the generalized sensitivity analysis approach prior to EKF analysis is suggested as a valuable approach, providing information on parameter indentification which can be used to reduce the estimation problem to a manageable level.

Acknowledgements—The authors are grateful to Peter Toms and Alan Steele of the Thames Water Authority for the provision of data and fruitful discussions and to Dr Enda O'Connell for useful comments on the manuscript. The views expressed in the paper are those of the authors and do not necessarily represent the views of the Thames Water Authority.

REFERENCES

Beck M. B. (1978) A comparative case study of dynamic models for DO-BOD-algae interaction in a freshwater river. IIASA Report RR-78-19.

Beck M. B. and Young P. C. (1976) Systematic identification of DO-BOD model structure. *Am. Soc. civ. Engrs Envir. Engng Div.* 102, 909-924.

Bowles B. A. (1978) Phytoplankton populations of the River Thames. Ph.D. Thesis, London University.

Fritsch F. E. (1902) Preliminary report on the phytoplankton of the Thames. *Ann. Bot.* 16, No. 43, 1-9.

Fritsch F. E. (1903) Further observations of the phytoplankton of the River Thames. *Ann. Bot.* 17, No. 48, 631-647.

Fritsch F. E. (1905) The plankton of some English rivers. *Ann. Bot.* 19, 163-167.

Hornberger G. M. and Spear R. C. (1980) Eutrophication in Peel Inlet—I. The problem defining behaviour and a mathematical model for the phosphorus scenario. *Water Res.* 14, 29-42.

Hornberger G. M. and Spear R. C. (1981) An approach to the preliminary analysis of environmental systems. *J. envir. Mgmt* 12, 7-18.

Jazwinski A. H. (1970) *Stochastic Processes and Filtering Theory*. Academic Press, New York.

Kowalczewski H. and Lack T. J. (1971) Primary production and respiration of the phytoplankton of the River Thames and Kennet at Reading. *Freshwat. Biol.* 1, 197-212.

Lack T. J. (1971) Quantitative studies on the phytoplankton of the River Thames and Kennet at Reading. *Freshwat. Biol.* 1, 213-224.

Lederman T. D., Hornberger G. M. and Kelly M. G. (1976) The calibration of a phytoplankton growth model using batch culture data. *Wat. Air Soil Pollut.* 5, 431-442.

Lund J. W. G. (1949) Studies of *Asterionella* (1). Origin and nature of cells producing seasonal maxima. *J. Ecol.* 37, 389-419.

Onstad C. A. and Blake J. (1980) Thames basin nitrate and agricultural relations. *Proceedings of ASCE Watershed Management Symposium*, Boise, Idaho.

Rice C. H. (1938) Studies in the phytoplankton of the River Thames 1 and 2. *Ann. Bot. N.S.* 2, 539-557; 559-581.

Spear R. C. and Hornberger G. M. (1980) Eutrophication in Peel Inlet—II. Identification of critical uncertainties via generalized sensitivity analysis. *Water Res.* 14, 43-49.

Steele J. A. (1978) Reservoir algal productivity. In *Mathematical Models for DO-BOD-Algae Interaction in a Freshwater River*. International Institute for Applied Systems Analysis. Report RR-78-19.

Swale E. M. F. (1962) Studies in the phytoplankton of a calcareous river. Ph.D. Thesis, University of London.

Thomann R. V. (1972) *Systems Analysis and Water Quality Management*. McGraw-Hill, New York.

Toms I. P., Mindenhall M. J. and Harman M. M. I. (1975) Factors affecting the removal of nitrate by sediments from rivers, lagoons and lakes. WRC Technical Report, TR114.

Whitehead P. G. (1980) An instrumental variable method of estimating differential equations of dispersion and water quality in non-tidal rivers. *J. Ecol. Model.* 9, 1-14.

Whitehead P. G. and Hornberger G. (1984) Modelling algal behaviour in the River Thames. In *Proceedings of Workshop "Water Quality Modelling, Forecasting and Control"* (Edited by Whitehead P. G. and O'Connell P. E.). Institute of Hydrology Report.

Whitehead P. G., Young P. C. and Hornberger G. (1979) A systems model of flow and water quality in the Bedford Ouse river system—I. Streamflow modelling. *Water Res.* 13, 1155–1169.

Whitehead P. G., Beck M. B. and O'Connell P. E. (1981) A systems model of flow and water quality in the Bedford Ouse river system—II. Water quality modelling. *Water Res.* 15, 1157–1171.

Whitehead P. G. and Williams R. J. (1982) A dynamic nitrate balance model for river basins. *IAHS Conference Proceedings*, IAHS publication 139.

Whitehead P. G., Caddy D. E. and Templeman R. F. (1983) An on-line monitoring, data management and forecasting system for the Bedford Ouse river system. *IAWPC Third River Basin Management Conference Proceedings*, York.

Young P. C. (1974) A recursive approach to time series analysis. *Bull. Inst. Appl.* 10, 209–224.

APPENDIX 6

QUASAR

QUAlity Simulation Along Rivers
Software from the Institute of Hydrology

QUASAR is a river network water quality and flow model developed for use on DEC VAX computers. The program has been designed to be easy to use with no requirement to understand the computer operating system (VMS) or the structure of data files. Output is in the form of colour graphics on screen or plotter, and in tabular form on printers.

Parameters modelled are flow, nitrate, dissolved oxygen, ammonia, temperature, E. Coli, pH, Biochemical Oxygen Demand and a conservative pollutant or tracer.

QUASAR software in operation.

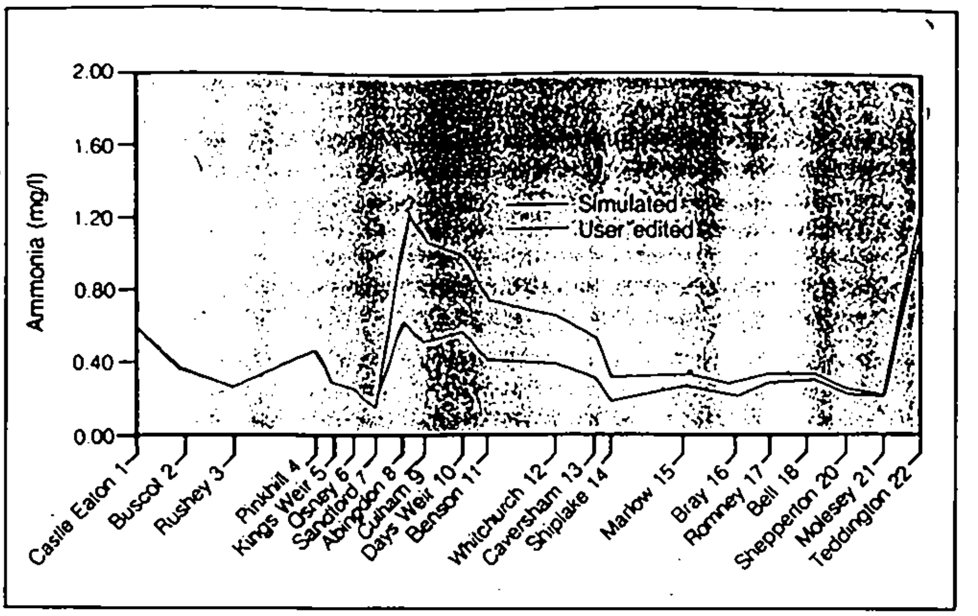
The QUASAR model is composed of a set of equations describing the changes in water quality and flow over time. In its dynamic mode, time series data are input to the model and flow and quality estimates are generated at each reach boundary over a period of time. Travel times are incorporated so that pollution pulses can be tracked downstream. In the planning mode a Monte Carlo simulation approach is used to provide distributions of flow and quality at key sites of interest. Effluent consent levels can be designed to meet River Quality Objectives.

Key features

- Drives DEC VT 100 class terminals and IBM PCs using terminal emulation.
- Entirely menu driven
- Data input from text (ASCII) files
- Interactive data preparation and editing using menus and forms
- Colour graphics
- Parameter sets hold descriptions of model runs
- Planning and dynamic (prediction) modes
- Runs in multi-user environment
- Easily adapted to other river systems
- 8 quality parameters and flow modelled

QUASAR models a river as a series of reaches usually defined by the locations of tributary confluences, weirs, public water supply intakes or effluent discharges. Each reach is subdivided into a number of subreaches each modelled as a stirred tank reactor. At the input to a reach a mass balance is performed on all the inputs or abstractions and the resulting river quality is routed down the reach.

During their passage through the reach the concentrations of the water quality parameters are modified according to instream physical and chemical processes. For example, in the case of dissolved oxygen, additions are made through reaeration and photosynthetic oxygen production and losses occur due to the decay of BOD, the nitrification of ammonia and the respiration of algae and river muds.



River profile predicting the downstream effects of an ammonia pollution event at Sandford on the Thames.

The QUASAR package

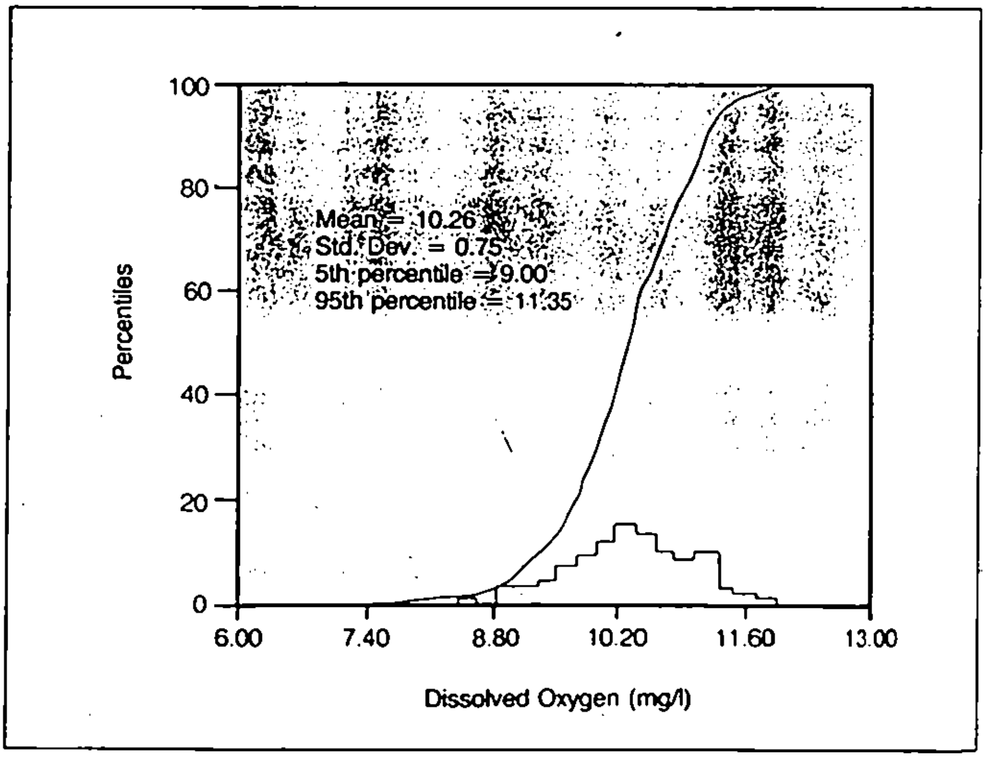
QUASAR currently runs on DEC VAX computers; an IBM PS/2 version is planned for release in 1990.

The following are required to run QUASAR:

- DEC VAX running VMS version 4.7 or later
- UNIRAS Graphics Library version 5.4 or 6.1
- At least 20,000 blocks of disk space (application dependent)
- DEC VT series terminal or compatibles (e.g. VT100, VT220 VT340 or IBM PC with terminal emulation)
- RETOS if VT340 colour graphics are to be displayed on an IBM PC using KERMIT
- Graphical output device(s) compatible with the local UNIRAS installation (e.g. DEC LA50, VT340)

QUASAR output

In dynamic mode the simulated water quality and flow can be viewed either as a profile along the river system or against time at any reach of interest (e.g. river abstraction site). In the planning mode cumulative frequency and distribution curves are generated at any point. Rapid graphical colour displays provide an efficient means of assessing the results of model runs.



Planning mode output showing distribution and frequency curve for dissolved oxygen at Gunnislake.

All Trade marks are acknowledged. If you require further information on QUASAR please contact:

INSTITUTE OF HYDROLOGY
Wallingford
Oxfordshire OX10 8BB
United Kingdom

Telephone: 0491 38800
Telex: 849365 HYDROL G
Fax: 0491 32256

Natural Environment Research Council

APPENDIX 7

The surface waters acidification programme

EDITED BY B. J. MASON

Director, UK–Scandinavian Surface Waters Acidification Programme, Centre for Environmental Technology, Imperial College of Science, Technology and Medicine, London

CAMBRIDGE UNIVERSITY PRESS

Cambridge
New York Port Chester
Melbourne Sydney

Modelling long-term trends in surface water acidification

By P. G. Whitehead[1], A. Jenkins[1] and B. J. Cosby[2]
[1] *Institute of Hydrology, Wallingford, Oxfordshire OX10 8BB, U.K.*
[2] *Department of Forestry, Duke University, North Carolina, U.S.A.*

To assess long-term acidification trends models are required that can characterize the principal mechanisms operating, account for the changing levels of deposition inputs and provide good estimates of past, present and future soil and water chemistry. At the same time the model should be transferable so that it can be readily applied to a wide range of catchments in differing pollution climates with differing land-use regimes and differing soils and parent geology. In this paper the application of MAGIC (model of acidification of groundwaters in catchments) is described for moorland and afforested catchment sites in Scotland and Wales. In addition, MAGIC has been applied in a regional analysis to predict distributions of water quality across Wales and the Galloway region of Scotland. The sensitivity of the model to parameter variations between sites is explored and the model used in a predictive mode to assess effects of land-use change such as afforestation and the likely changes in future atmospheric pollutant deposition levels.

The model results support the findings of palaeoecological studies that acidification has occurred in many U.K. catchments and demonstrates a clear link between deposition of atmospheric pollutants and acidification.

1. Introduction

Acidification may be regarded as essentially a problem over two very different timescales. Short-term fluctuations in acidification are generally driven by meteorological factors and hydrological processes operating in the catchment. The timescale of these events are in the order of hours, or at most days, and the level of acidity will be largely controlled by the ability of the catchment to buffer incoming acidity within the catchment's hydrological response time. On the other hand, long-term changes in soil and water chemistry can occur over years or decades causing chronic acidification.

Approaches to short-term response modelling are described elsewhere (Christophersen *et al.* 1982; Whitehead *et al.* 1986*a*, *b*; Wheater *et al.*, this symposium). Modelling long-term changes in acidification has been approached in two ways. The first is an empirical approach whereby extrapolations from present conditions are made by using empirical relations between rainfall chemistry and surface water quality (Henriksen 1979). The second approach utilizes mechanistic, process-orientated, numerical models of hydrology and geochemistry to make the quantitative linkage between deposition and water quality (Schnoor *et al.* 1984; Seip & Rustad 1983; Cosby *et al.* 1985*a*, *b*). It is essential that such models take into account the long-term interactions occurring between physical and chemical characteristics within a catchment and can account for the dominant processes operating. In this paper we describe one such model, MAGIC (model of acidification of groundwaters in catchments) and illustrate its application to Wales and Scotland. Results from specific sites are presented in addition to a regional analysis. The model is used in a predictive manner to assess the effect of different future pollutant deposition patterns and the impacts of land-use change such as afforestation. An analysis of the calibrated model parameters from a variety of sites is considered.

2. Conceptual basis of MAGIC

Extensive details of the background theory and equations used in MAGIC have been given by Cosby *et al.* (1985*a*). However, the dominant processes incorporated include.

1. Anion retention by catchment soils (e.g. sulphate adsorption).
2. Adsorption and exchange of base cations and aluminium by soils.
3. Alkalinity generation by dissociation of carbonic acid (at high carbon dioxide partial pressures in the soil) with subsequent exchange of hydrogen ions for base cations.
4. Weathering of minerals in the soil to provide a source of base cations.
5. Control of Al^{3+} concentrations by an assumed equilibrium with a solid phase of $Al(OH)_3$.

MAGIC simulates these processes by using the following.

1. A set of equilibrium equations which quantitatively describe the equilibrium soil processes and the chemical changes that occur as soil water enters the stream channel.
2. A set of mass balance equations which quantitatively describe the catchment input–output relationships for base cations and strong acid anions in precipitation and stream water.
3. A set of definitions which relate the variables in the equilibrium equations to the variables in the mass balance equations.

3. Application to the Allt a'Mharcaidh – a moorland transitional site

The Allt a'Mharcaidh is a transitional site located in the Cairngorm Mountains of NE Scotland. Full details of catchment characteristics, instrumentation and sampling methodology are given elsewhere (Jenkins *et al.* 1988; Ferrier & Harriman, this symposium).

MAGIC has been applied to the catchment by using a two-stage optimization procedure. First, the nitrate and ammonia uptake rates are determined together with the soil-sulphate adsorption capacity. These parameters are all independent and therefore can be optimized to give a unique value to match the output stream chemistry. The second stage of the optimization considers the parameters controlling cation behaviour, namely weathering rates, which control cation supply from bedrock, and selectivity coefficients, which control ion exchange in the soils. The output stream chemistry and measured base saturation are used to drive the Rosenbrock optimization procedure, a robust and generally reliable technique. Full details of the optimization of model parameters are given by Jenkins *et al.* (1988) and a comparison of model parameters in relation to other site applications of MAGIC are given later in this paper (see table 4).

Table 1. *Observed and simulated stream chemistry for the Allt a'Mharcaidh* (in microequivalents per litre)

	1846 model simulated	1986 model simulated	1986 observed	2126 model simulated
Ca	21.4	37.5	37.1	43.8
Mg	28.6	29.6	29.9	29.7
Na	102.1	117.0	116.1	115.1
K	7.9	8.9	8.4	10.2
NH_4	0.0	2.0	—	2.2
SO_4	15.2	50.3	50.1	70.0
NO_3	0.0	2.2	2.1	2.2
Cl	111.3	111.3	111.3	111.3
Alk	33.5	31.6	33.0	17.2
H	1.6	1.7	2.0	2.8
pH	5.8	5.8	5.7	5.6

MAGIC produces a close match between observed and simulated stream chemistry as shown in table 1. Simulated soil base saturations are also good estimates of observed values at 8%. Historical reconstruction and future response, assuming constant deposition chemistry at current levels to 2126, are also shown in table 1.

In the Allt a'Mharcaidh catchment, soils have retained a high buffering capacity since 1846 with almost unchanged alkalinity and pH in streamwater. By 2126, however, assuming constant deposition into the future, a decrease in alkalinity to *ca.* 30% of the present value is forecast with a drop in mean pH of only 0.1 unit. Stream sulphate levels increase steadily from 1846 to the present day and continue to rise to 2126. Soil base saturation remains almost constant to the present, despite increased output of base cations, due to high weathering rates. Base saturation deteriorates beyond 1986, however, as soil exchange sites become saturated with hydrogen and strong acid anions.

The simulation results differ markedly from the pattern of change demonstrated by the MAGIC simulation of Dargall Lane, a heavily acidified catchment in SW Scotland (Cosby *et al.* 1986). In particular, sulphate concentrations in streamwater at the Allt a'Mharcaidh do not reflect changes in the deposition sequence and the pH response is smooth and damped at this site. This is a direct consequence of the high value of E_{mx}, the maximum sulphate adsorption rate, that allows a high degree of sulphate adsorption and a long time-lag between any change of input chemistry and its resulting effect on output chemistry. Conversely, at Dargall Lane little sulphate adsorption has occurred so that any change in sulphate deposition is reflected almost immediately in the run-off chemistry. By keeping all optimized parameters and deposition factors constant, and running the hindcast and forecast simulation for different values of E_{mx}, a variety of responses can be produced and these are shown in figure 1*a*. As E_{mx} is decreased, response time decreases and input and output chemistry become similar, whereas increasing sulphate adsorption causes an attenuated sulphate response. A key parameter controlling acid inputs to the catchment is the sulphate dry-deposition factor. This increases the sulphate loading to the catchment to account for aerosol and dry deposition of anthropogenically derived sulphate. Estimating the value of this parameter is particularly difficult and the sensitivity of the Allt a'Mharcaidh to the parameter is illustrated in figure 1*b*.

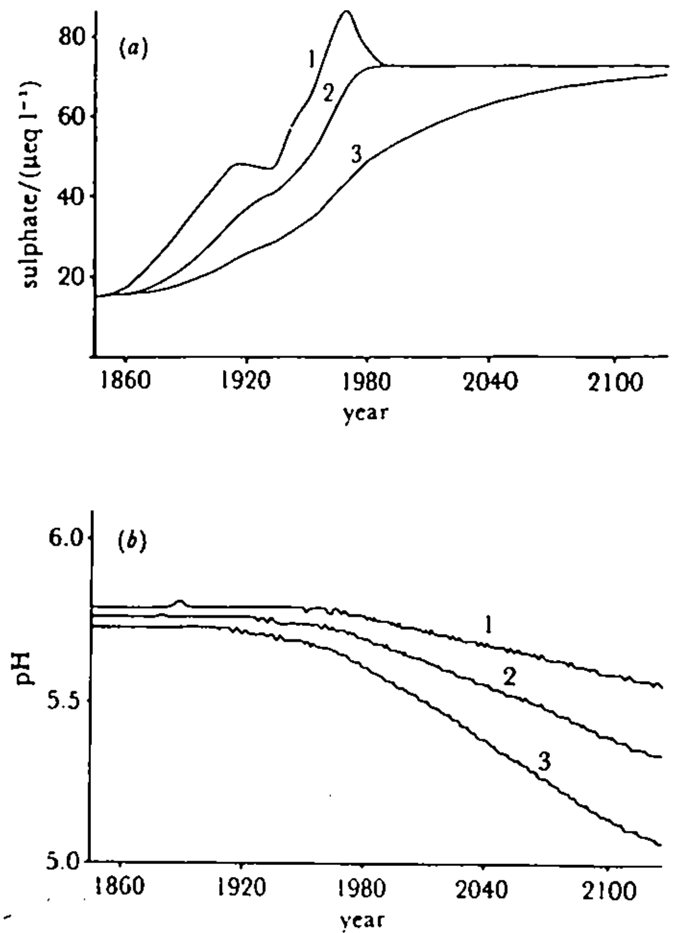


Figure 1. (a) Simulated stream sulphate concentrations assuming E_{mx}, the maximum sulphate adsorption rate, is 1.0, 10.0 and 28.6 for 1, 2 and 3, respectively. (b) Simulated pH showing the effect of enhanced dry deposition of sulphate. Dry deposition is 20%, 40% and 60% of wet deposition for 1, 2 and 3, respectively.

The higher the dry-deposition factor, the larger the pH decline. The major change in the pH trend occurs between 1980–1990 suggesting that the Allt a'Mharcaidh is a truly transitional site that will undergo faster acidification in the future if deposition remains at present-day levels. The rate of decline is highly dependent on aerosol deposition rates, which can be significant at the higher altitudes.

4. Application to Chon and Kelty – acidified catchments in central Scotland

MAGIC has been applied to the Chon and Kelty catchments, two forested sites, located in an area of high deposition 40 km north of Glasgow. Final optimized values of weathering rates and soil exchange selectivity coefficients are compared with other catchments later in this paper (see table 4). Values of weathering of calcium and magnesium are higher in Chon and this accords well with field observation of a dolerite dyke within the catchment that affects the outflow concentrations of these ions. Simulated stream chemistry (table 2) matches observed chemistry closely at both Chon and Kelty. The model also successfully simulates present-day soil

Table 2. *Observed and predicted present day stream chemistry at Chon and Kelty* (in microequivalents per litre)

	Chon		Kelty	
	observed	predicted	observed	predicted
Ca	43.3	45.7	19.0	20.6
Mg	48.3	46.2	36.9	36.0
Na	181.3	184.1	200.9	199.8
K	7.1	8.2	7.8	8.2
NH_4	7.2	6.9	13.2	12.9
SO_4	93.3	102.7	100.0	105.2
Cl	224.5	217.6	216.5	214.7
NO_3	3.0	2.9	10.2	10.1
Al_3	24.4	19.5	48.8	48.2
H	24.5	24.2	95.5	88.9
pH	4.6	4.6	4.0	4.1

chemistry as soil base exchange fractions at the two sites are well matched with measured data (Jenkins *et al.* 1990).

Stream pH, hydrogen ion, alkalinity, calcium and sulphate reconstructions for the two sites from 1847–1987 are shown in figure 2. Chon shows a very low background hydrogen ion concentration with an increasing trend which accelerates in the period 1950–1960 to give a rapid increase in hydrogen ion concentrations. Kelty shows a similar accelerated increase during that period but has a very high background concentration. This is because of the high level of organics in the catchment that are assumed to be at a constant level throughout the simulation. The period of rapidly increasing hydrogen corresponds to the planting and growth of the forest. At the time of canopy closure (1965), both catchments are subject to the most severe acidifying processes: (i) total load of anthropogenic wet and dry deposition is at a high level as the assumed deposition curve peaks at this time; (ii) input from canopy filtering is also at a maximum because canopy closure (and thus maximum filtering by the trees) and maximum deposition coincide; (iii) maximum cation uptake coincides with canopy closure; and (iv) the effect of increased evapotranspiration is also at a maximum. Around 1970 stream concentrations level off and by 1980 have started to decrease. This is in response to the falling deposition levels in recent years and to the decrease in uptake of base cations as the forest matures. This apparent recovery is in accord with reconstructions from diatom evidence (Battarbee 1988).

The base saturation reconstruction (figure 2*e*) indicates a progressive soil acidification through time as base cations are leached in response to the incoming acidity. High weathering rates at Chon produce a high initial base saturation although this falls steadily until 1950 and then accelerates downwards at the onset of afforestation. At Kelty, although the apparent initial base saturation is not as high as at Chon. The model indicates that cation losses from the soil will result in slightly higher percentage base saturation. No recovery of base saturation is seen at either site in response to decreased emissions since 1970, although the rate of decrease slows, and this accords well with the expected slower recovery of soils as they continue to desorb sulphate.

The effect of forest growth at the two sites is to accelerate acidification of the surface water as the result of a gradual increase in anthropogenic deposition. Similar

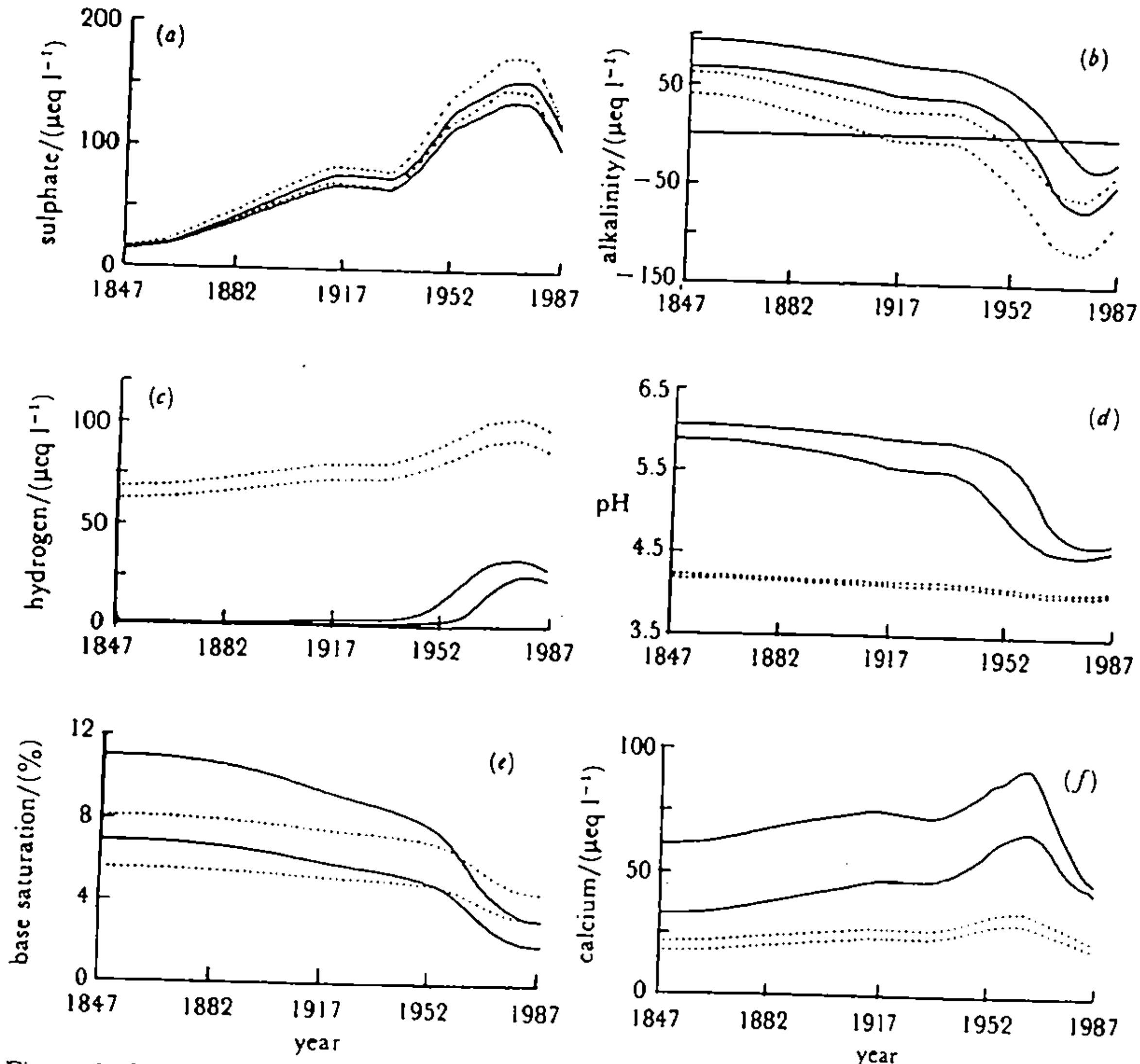


Figure 2. Simulated stream chemistry and soil base saturation for the Chon and Kelty sites in central Scotland; (---------) represent Kelty; (————) represents Chon, double lines represent the upper and lower ranges of expected behaviour.

results have been obtained previously by Whitehead *et al.* (1988*a*, *b*) for forested catchments in Wales at Plynlimon and Llyn Brianne. It should be emphasized that forests growing in pristine areas will not have such an acidifying effect as demonstrated by Neal *et al.* (1986). The model clearly demonstrates that as well as the effects of canopy interception, evapotranspiration and cation uptake cause a significant acidification of the soil. This can in turn cause enhanced surface water acidification depending on the activity of the mobile anion and the base cation status of the soil. At Kelty the increased soil acidification appears to lead to water acidification because hydrogen is removed from the soil associated with sulphate, whereas at Chon, base cations are exchanged thereby affording some buffer to the stream acidity.

5. Regional application of MAGIC to Wales

MAGIC has been applied in a regional context to assess water quality changes across a range of streams or lakes. In the regional approach, the MAGIC is run repeatedly

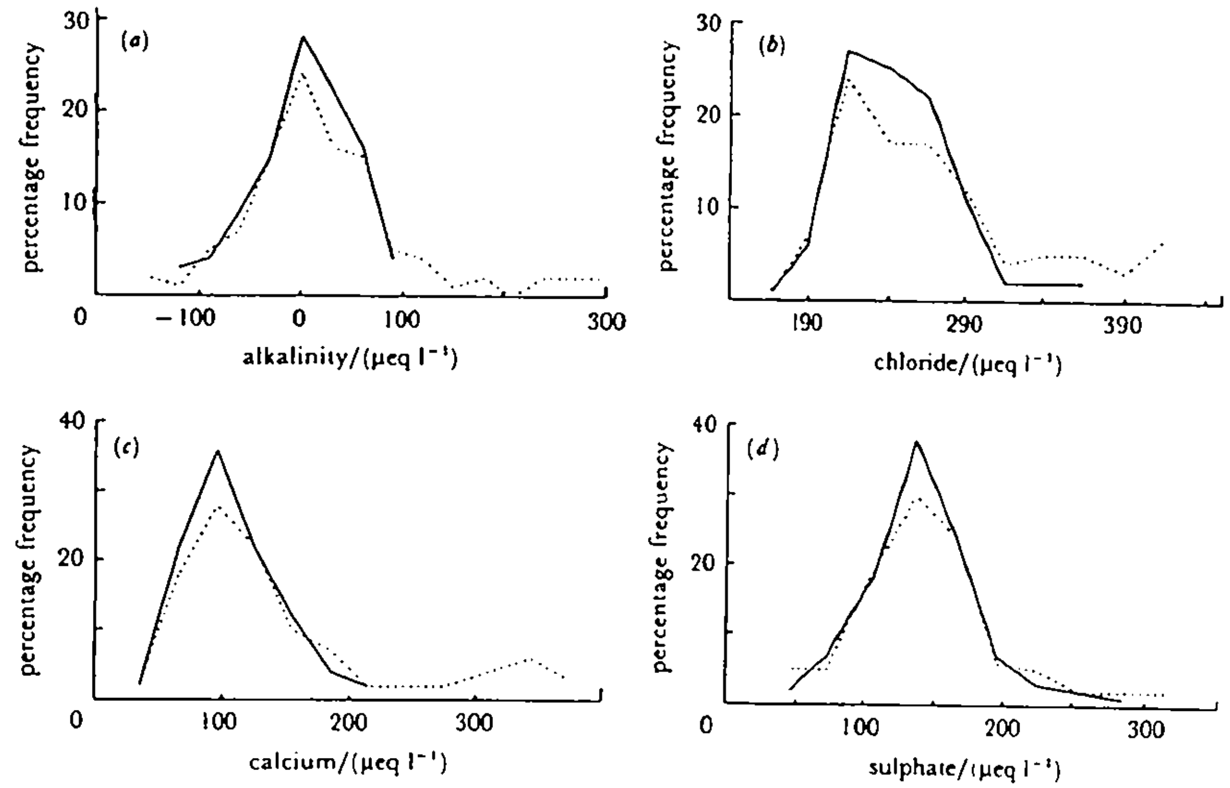


Figure 3. Observed (···) and simulated (——) stream chemistry distributions for Wales using the full observed regional data set; (*a*) alkalinity, (*b*) chloride, (*c*) calcium and (*d*) sulphate.

with different parameter values chosen randomly from given distributions. The ensemble of model runs is then evaluated and compared with the observed distributions of water quality across the region obtained from analysis of survey data. This Monte Carlo approach allows a simulation of the water quality changes across the region as a whole. The approach was developed by Cosby *et al.* (1988) and Hornberger *et al.* (1989) in an analysis of 700 Norwegian lakes. A similar approach has been used by an analysis of surface water in the Galloway region of Scotland (Musgrove *et al.* 1990) and in Wales by Jenkins *et al.* (1990).

Figure 3 shows the simulated distribution of calcium, magnesium, alkalinity and sulphate against the observed distributions for Wales obtained from 130 streams. In all cases the simulated distribution is close to the observed distribution suggesting that the model has captured the principal features of water quality across the region. Of particular interest is the question of how the water quality distributions in the region have changed over time. As shown in figure 4, the pre-industrial 1844 distributions for sulphate and alkalinity are very different from the present day. Sulphate levels are much lower and alkalinity is significantly higher. The temporal changes in the entire regional distributions have also been investigated under an assumed 30% deposition reduction in excess sulphate deposition linearly between present day and the year 2000. Although sulphate chemistry in the streams is reduced, there is no major shift in alkalinity. This is probably because the base saturation levels of the soils are low and even a 30% reduction in sulphate is insufficient to achieve a significant recovery on the base-poor Welsh soils.

The portion of the simulated region that has alkalinity less than zero was subjected to various hypothetical future deposition patterns in an attempt to look at the likely

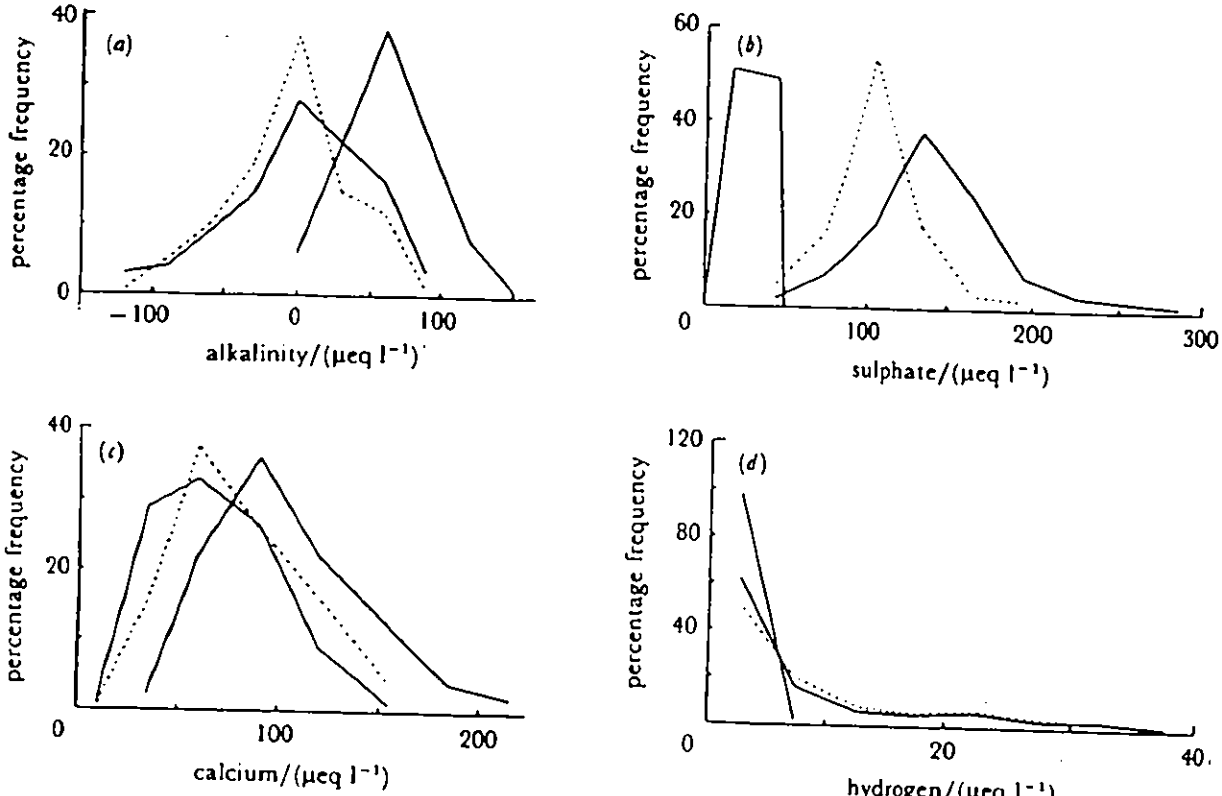


Figure 4. Simulated background (—), present day (——) and future (···) stream chemistry for Wales assuming a 30 % decrease in acid deposition; (a) alkalinity, (b) sulphate, (c) calcium and (d) hydrogen.

response of the worst affected sites. Three future deposition scenarios were used, linear reduction in non-marine sulphate deposition over a 20 year period to 30 %, 60 % and 90 % of the 1984 value, thenceforth remaining constant. Table 3 describes the predicted chemistry equlibria for each deposition scenario. The major feature of the results is the trend in increased pH and alkalinity and decreased sulphate in the streams as the deposition is decreased. Reductions in deposition of 30 % and 90 % lead to mean stream sulphate concentrations of 115 and 43.7 μequiv l^{-1}, respectively. This reduction of sulphate concentrations raises alkalinity, from a mean of 9.4 to 75.2 μequiv l^{-1}. Coupled with the change in alkalinity, the pH rises from a mean of 5.5–6.2. Ormerod (1989) assessed changes from a biological viewpoint and suggested that trout survival in Welsh streams would be significantly improved with a 60 % reduction in sulphate deposition.

6. Regional application of MAGIC to southwest Scotland

The Galloway Region of SW Scotland contains many lochs and streams that drain moorland, forest and pasture catchments. The bedrock consists mainly of lower palaeozoic rocks of Ordovician and Silurian age with a few intrusions of granite of the Old Red Sandstone age. The Galloway region differs significantly from Wales in that it is an area of high deposition and has many acidified lakes. MAGIC has been applied to Galloway using the same procedure as for Wales. As is the case for Wales a close fit is obtained between the observed and simulated water quality distributions for Galloway. The changes over time in the distributions of simulated chemistry were

Table 3. *Welsh stream concentrations in equilibrium with reduced deposition for 10% most sensitive sites*
(in microequivalents per litre)

variable	mean	standard deviation	minimum	maximum
		(*a*) effect of a 90% reduction in deposition		
pH	6.2	0.2	5.6	6.5
Na	230.4	43.2	146.8	322.0
Ca	68.7	27.8	25.8	149.0
Mg	62.3	14.0	36.86	106.3
SO_4	43.7	6.4	34.5	58.5
Cl	253.8	47.2	168.9	347.1
Alk	75.2	32.0	14.5	150.7
		(*b*) effect of a 60% reduction in deposition		
pH	5.9	0.3	5.1	6.3
Na	231.5	42.8	154.5	322.0
Ca	26.8	26.8	28.0	149.0
Mg	64.8	13.7	40.3	107.1
SO_4	79.8	12.9	58.4	106.9
Cl	253.8	47.2	168.9	347.1
Alk	43.9	25.8	−6.9	96.6
		(*c*) effect of a 30% reduction in deposition		
pH	5.5	0.4	4.7	6.0
Na	231.9	42.4	159.2	322.0
Ca	71.8	26.4	28.8	149.0
Mg	65.8	13.6	41.4	107.2
SO_4	115.8	21.3	80.1	161.3
Cl	253.8	47.2	168.9	347.1
Alk	9.4	23.7	−59.9	44.6
		(*d*) current chemistry		
pH	5.1	0.4	4.9	5.3
Na	236.6	41.3	167.0	333.1
Ca	79.2	23.4	41.9	147.6
Mg	76.4	19.1	47.0	138.7
SO_4	153.2	30.2	98.4	216.8
Cl	253.8	47.2	168.9	347.1
Alk	−4.9	3.6	−11.9	0.4

ascertained by investigating the output for 1844, 1982 and 2060. The future deposition was modelled as a linear decrease to 30% of the 1982 level by the year 2001 and constant thereafter. The results are presented in detail by Musgrove *et al.* (1990) and model reconstruction shows a large drop in both pH and alkalinity over the past 140 years. The pH level falls by 0.8 pH unit and alkalinity falls by *ca.* 70 μequiv l^{-1}. This is in accord with the findings of Battarbee & Flower (1985), who report changes in pH level up to 1.0 pH unit during the same period, for those lochs in the granitic region of Galloway. Very little recovery is seen during the future scenario. The small size of this recovery reflects the depletion in the soil of base cations with the low rate of soil weathering in the region, that enable only a slow recovery rate. Alkalinity levels indicate a major shift in distribution from 1840 levels to current values. Even with a further 30% reduction in sulphate deposition alkalinity shows no major shift and indicates the scale of the problem across a sensitive region such as Galloway.

Table 4. *Parameter values for a range of* MAGIC *applications*

Site – location	E_{mx} [a]	weathering rates [b]				selectivity coefficients [c]				reference
		Ca	Mg	Na	K	Ca	Mg	Na	K	
Allt a'Mharcaidh – Scotland	28.9	29.2	12.1	11.1	9.9	3.02	3.18	−0.28	−3.64	Jenkins *et al.* 1988
White Oak Run – U.S.A.	8.0	0.0	10.0	4.0	12.0	4.1	4.1	−0.5	−1.01	Cosby *et al.* 1985
Dargall Lane – Scotland	0.1	38.0	35.0	2.0	8.0	2.49	2.91	−0.22	−3.92	Cosby *et al.* 1986
Lake Gardsjon – Sweden	1.0	10.0	12.0	13.0	2.0	1.9	4.1	0.7	−1.0	Wright *et al.* 1986
Lake Hovvatn – Norway	1.0	3.0	1.0	0.5	0.5	1.0	2.2	−0.5	−4.0	Wright *et al.* 1986
Llyn Brianne – Wales	0.01	25.0	15.0	10.0	1.0	1.94	1.67	−2.1	−5.33	Whitehead *et al.* 1988
Plynlimon – Wales	3.38	116.9	88.2	66.4	0.0	2.70	3.27	−0.65	−4.70	Whitehead *et al.* 1988
Loch Chon – Scotland	7.0	53.0	58.0	8.0	10.0	1.16	2.22	0.28	−3.42	Jenkins *et al.* 1990
Loch Tinker – Scotland	4.4	110.0	22.0	5.0	1.0	0.06	−0.69	−0.69	−3.91	Jenkins *et al.* 1990
Yli Knuatila – Finland	1.5	17.0	10.5	1.8	1.8	2.4	4.21	0.60	−3.63	Lepisto *et al.* 1988
Kelty Water – Scotland	3.5	1.0	17.0	27.0	14.0	−0.82	0.77	0.07	−3.62	Jenkins *et al.* 1990

[a] In milliequivalents per kilogramme.
[b] In milliequivalents per square metre per annum.
[c] log S (Al cation).

7. Transferability of MAGIC

MAGIC has now been applied to 26 individual sites, two plot experiments (Wright 1987; Skeffington, personal communication) and in several regional analyses in the U.K. (Scotland and Wales), in Norway and extensively in the U.S.A. Table 4 shows a typical range of applications of MAGIC together with key parameters such as E_{mx}, (the maximum sulphate adsorption capacity of the soils) weathering rates and selectivity coefficients. As might be expected with the highly heterogeneous nature of geology, soils, vegetation and hydrochemical flowpaths in catchments, parameters vary from site to site. For example E_{mx} is particularly high at the Allt a'Mharcaidh and White Oak Run reflecting the sulphur adsorbing properties of soils in these catchments. Also weathering rates vary from site to site and reflect solid and drift geology. Loch Chon shows high weathering rates and this arises from a doleritic dyke in the catchment providing a significant source of base cations from weathering reactions. Similarly, Plynlimon shows high weathering rates in the moorland catchment reflecting liming that occurred over 40 years ago. Selectivity coefficients also vary from site to site but provide a consistent set of values.

8. Conclusions

MAGIC has been applied to a range of sites in Scotland and Wales and comparison with palaeocological results suggest that it gives a good representation of the long-term behaviour of catchments (Jenkins *et al.* 1990). Its wide application to many sites in Scandinavia, North America and the U.K. support this view as does the regional application in Wales and southwest Scotland.

The program confirms that acidification of surface water is a serious problem in some parts of Britain. Acidification levels are high in areas with thin base-poor soils on granitic type geology. Unfortunately, afforestation in high deposition areas tends to enhance the acidity by scavenging or filtering acidic particles and mist and this effect can be very significant often doubling the loads of acidic deposition entering catchments. It should be emphasized that afforestation in low deposition regions appears to have minimal effect (Neal *et al.* 1988). However, a strategy for forestry management to minimize acidification effects is still required for Scotland.

Although acidification appears to be at least partly reversible the MAGIC model indicates that significant levels of emission reductions are required for there to be a sustained recovery. Different catchments will show different reversibility responses dependent on factors such as soil-base, saturation levels, sulphate adsorption and release mechanisms, weathering rates, hydrological flow paths and deposition rates. Although there are many uncertainties in the model, it provides the only means at present of making site specific or regional predictions of long-term future behaviour of stream and lake acidity.

The authors are indebted to staff of the Institute of Hydrology for their technical support throughout SWAP and to the SWAP Committee for providing funding and support over the past four years.

References

Battarbee, R. W., Flower, R. J., Stevenson, A. C., Jones, V. J., Harriman, R. & Appleby, P. G. 1988 *Nature, Lond.* 332, 530–532.

Battarbee, R. W., Flower, R. J., Stevenson, A. C. & Rippey, B. 1985 *Nature, Lond.* 314, 350–352.

Christophersen, N., Seip, H. M. & Wright, R. F. 1982 *Wat. Resour. Res.* **18**, 977–997.

Cosby, B. J., Hornberger, G. M. & Wright, R. F. 1988 In *Uncertainty and regional modelling* (ed. J. Kamari), Reidel. (In the press.)

Cosby, B. J., Whitehead, P. G. & Neale, R. 1986 *J. Hydrol.* **84**, 381–401.

Cosby, B. J., Wright, R. F., Hornberger, G. M. & Galloway, J. N. 1985*a* *Wat. Resour. Res.* **21**, 51–63.

Cosby, B. J., Wright, R. F., Hornberger, G. M. & Galloway, J. N. 1985*b* *Wat. Resour. Res.* **21**, 1591–1601.

Henriksen, A. 1979 *Nature, Lond.* **278**, 542–545.

Hornberger, G. M., Cosby, B. J. & Wright, R. F. 1989 *Wat. Resour. Res.* **25**, 2009–2018.

Jenkins, A., Ferrier, R. C., Walker, T. A. B. & Whitehead, P. G. 1988 *Wat. Air Soil Pollut.* **40**, 275–291.

Jenkins, A., Whitehead, P. G., Musgrove, T. J. & Cosby, B. J. 1990 *J. Hydrol.* (In the press.)

Lepisto, A., Whitehead, P. G., Neal, C. & Cosby, B. J. 1988 *Nordic. Hydrol.* **19**, 99–120.

Musgrove, T. J., Whitehead, P. G. & Cosby, B. J. 1990 In *Impact models to assess regional acidification* (ed. J. Kamari), pp. 131–135. Amsterdam: Kluwer.

Neal, C., Whitehead, P. G. & Cosby, B. J. 1986 *J. Hydrol.* **84**, 381–401.

Ormerod, S. J., Weatherley, N. S., Varallo, P. V. & Whitehead, P. G. 1988 *Freshwat. Biol.* **20**, 127–140.

Schnoor, J. L., Palmer, W. D. & Glass, G. E. 1984 In *Modelling of total acid precipitation impacts* (ed. J. L. Schnoor), vol. 9, pp. 155–173. Boston: Butterworth.

Seip, H. M. & Rustad, S. 1983 *Wat. Air Soil Pollut.* **21**, 217–223.

Whitehead, P. G., Neal, C., Seden-Perriton, S., Christophersen, N. & Langan, S. 1986*a* *J. Hydrol.* **85**, 281–304.

Whitehead, P. G., Neal, C. & Neale, R. 1986*b* *J. Hydrol.* **84**, 353–364.

Whitehead, P. G., Bird, S., Hornung, M., Cosby, B. J., Neal, C. & Paricos, P. 1988*a* *J. Hydrol.* **101**, 191–212.

Whitehead, P. G., Reynolds, B., Hornung, M., Neal, C., Cosby, B. J. & Paricos, P. 1988*b* *Hydrol. Process.* **2**, 357–368.

Wright, R. F., Cosby, B. J., Hornberger, G. M. & Galloway, J. N. 1986 *Wat. Air Soil Pollut.* **30**, 367–380.

Wright, R. F. & Cosby, B. J. 1987 *Atmos. Environ.* **21**, 727–730.

Discussion

M. Cresser (*Aberdeen University, Department of Plant and Soil Science, Old Aberdeen, Scotland, U.K.*). I would like to return to the very important point raised by Sir John Mason about the reliability of MAGIC for making long-term predictions. It is often not clear precisely where the numbers inserted in some of the numerous black boxes of the model come from. Could Dr Whitehead confirm that often such numbers are selected from within a wide range of possible values to make the predicted water solute composition fit the observed data? If this is so, is it not possible that some key processes (especially biological processes) may be being ignored completely? Could this not substantially limit the validity of some of the conclusions reached about long-term effects?

P. G. Whitehead. First, MAGIC is a process-based model rather than a black-box model. Key processes are included in the model are ion exchange, weathering, CO_2 degassing, sulphate adsorption, etc. Most of these are chemical processes. Biological processes are not included explicitly because there is still considerable debate as to what biological controls are operating and to what extent they influence stream and soil chemistry. Organic acid is included in the model as are temperature effects. I do not feel that any major processes are missing in MAGIC or else this model could not reproduce the chemistry in so many different sites or regions. Hence I do not believe the major conclusions concerning long-term effects are invalid. Indeed all the field evidence is that reversibility predicted by MAGIC is already occurring.

APPENDIX 8

PESTICIDE TRANSPORT MODELLING

Pesticide Transport Modelling

The model structure presented here is derived from detailed measurements of soil water movement and distribution made at experimental sites over successive winters by members of the Agrohydrology section of the Institute of Hydrology (Bell *et al*), 1991 and 1992). Broadly an underdrained field consists of two types of soil profile characterised by the rate at which they allow downward water movement. The bulk of the soil in the inter-drain position has a very low hydraulic conductivity which approaches zero when the soil is saturated; downward water movement through the soil matrix is therefore very slow. The soil above the drains seems to have a much higher hydraulic conductivity and thus water movement through the soil matrix in this part of a field is much quicker. thus once the soil below the drains is saturated and they begin to flow the hydrological response of the drain is controlled by the soil immediately above and adjacent to the drains.

A diagrammatic representation of the model is shown in figure 1. The model considers the top 2 m of the soil profile which is divided into three layers above the level of the drains and one below. Above the drain the layers are divided into two to represent the fast and slow parts of the soil profile described above. The slow portion of the field is considered to be up -slope of the fast part and the subsequent possible directions of water movement are shown by the arrows in figure 1. The dotted arrows indicate the possibility of water moving directly to lower layers without interacting with intervening layers via macropores and/or cracks. The transport of pesticide in the system is assumed to be associated with the water movement, the pesticide being partioned between the soil and water phases at the end of each timestep. The model keeps account of the amount of water and dissolved and absorbed pesticide in each box and calculates changes to these depending on a mass balance of inputs, outputs and internal sources and sinks.

To explain the details of water and pesticide movement it is best to consider a single box from the model (Fig 2).

Water Movement

The change in soil water content of box i, S_i is given by;

$$\frac{dS_i}{dt} = q_{i-1} - qbp_i + d_u - q_i - d_i + qbm_{i-1}$$

where q_i is the flow per unit (mm) area from box i, d_u is the flow per unit area (mm) from an up-slope box, d_i is the flow to a down-slope box or stream, qbp_i is the flow from box i-1 that by-passes box i in cracks or macro-pores, qbm_{i-1} is the flow that was in by-pass routes in box i-1 that return to the soil matrix in box i and t is time (hours). Flow may only occur from box i, either vertically, q_i or laterally, d_i when $S_i > SFC_i$, where SFC_i is the field capacity of box i. Flow from box i depends on the water content of box 1 and is given by;

$$q_i = k_v(S_i - SFC_i)(1-\tan(\alpha))$$

where k_v (hours^{-1}) is a measure of the vertical conductivity of box i, and α is the average slope of the field. Similar the down slope drainage d_i is given by;

$$d_i = k_h(S_i - SFC_i)\tan(\alpha)$$

where k_h is a measure of the horizontal conductivity of box i. A fraction of water may by-pass a given layer through macro-pores and cracks. The fraction of by-pass flow through a box is related to the soil water content of the box, such that the drier the box the more by-pass flow can occur. This feature of the model is to take some account of the swelling nature of the soil. The by-pass flow fraction CF_i is given by;

$$CF_i = CFMIN_i + G_i(S_i - SMIN_i)$$

where

$$G_i = (CFMIN_i - CFMAX_i)/(SMAX_i - SMIN_i)$$

where $CFMIN_i$ is the minimum bypass flow fraction occuring at maximum water content, $SMAX_i$ and $CFMAX_i$ is the maximum bypass flow fraction occurring at minimum soil water content $SMIN_i$. Therefore,

$$qbp_i = CF_i q_{i-1}$$

The continuity of cracks through layers is given by the ratio, CF_i/CF_{i-1} to a maximum of unity. Thus once in a crack water is assumed to remain there until the crack ends. Hence,

$$qbm_i = \left(1 - \frac{CF_i}{CF_{i-1}}\right) qbp_{i-1}$$

Water may only enter a box if it is not saturated ie $S_i < SMAX_i$. $SMAX_i$ is given by;

$$SMAX_i = \theta_i V_i$$

where θ_i and V_i are respectively the porosity and volume (mm) of box i.

Pesticide Movement

Pesticide is added to the model by assuming that the amount applied is well mixed into the top layer of the model (boxes 1 and 5, Fig 1) and partioned following a reversible instantaneous linear absorption isotherm,

$$PS_i = PW_i Kd_i$$

and

$$k_i = k_{oc} OC_i$$

where PS_i is the pesticide concentration in the soil phase, PW_i is the concentration of the dissolved phase, kd_i is the absorption coefficient, k_{oc} is the absorption coefficient normalised for organic carbon content, OC_i.

The rate of change of mass of dissolved pesticide in the ith box, $S_i PW_i$ is given by,

$$\frac{dS_i PW_i}{dt} = (q_{i-1} - qbp_i)P_{i-1} + d_u PW_u - (q_i + d_i)P_i + qbm_{i-1}PW_{bm} - R_d PW_i$$

where, P_i is the pesticide concentration per unit area of the ith box (µg/mm), P_u is the pesticide concentration of water draining from an up-slope box, P_{bm} is the concentration of pesticide in the bypass flow and Rd is the first order rate coefficient describing degradation of the pesticide. Water moving through by-pass routes is assumed to have the same concentration as the soil water in the box with which it was last in contact. The rate of change of mass of pesticide absorbed onto the soil is given by;

$$\frac{dPS_i}{dt} = - R_d PS_i$$

where, P_i is the soil absorbed pesticide concentration per unit area in the ith box (µg/kg/mm^2). The degradation rate of the pesticide is assumed to be the same in both the liquid and solid phase. At the end of each model time step the pesticide is repartitioned between the soil and the soil water using the linear isotherm described above.

Drainflow

The model only allows drainflow when the deep soil box, (box 4, Fig 1) is at saturation. When this occurs drainflow is the sum of the vertically draining water from boxes 3 and 7 plus any water from rainfall and boxes 5 and 6 moving via by-pass routes. Water moving from boxes 3 and 7 is assumed to produce drainflow by displacement of water from box 4, while water in bypass routes is directly intercepted by the drain. The concentration of pesticide in the drainflow is thus a mass balance of the contributions from the various flow paths.

Stream Flow

Stream flow is the sum of the lateral drainage from each of the boxes, overland flow and drain flow. Again the concentration of pesticide is amass balance of the contributions from all the flow paths. Overland flow is generated when rainfall exceeds evaporation an either box 1 or box 2 are saturated. Water flowing overland from box 1 may infiltrate into box 5 if this box is not saturated. The concentration of pesticide in the surface runoff is assumed to be equal to the concentration of the box from which it was generated.

Model Application

The model has been applied over the period from the 1 Sep. 1990 to 31 Mar. 1991 but at this stage has only been used to simulate flow and isoproturon from the drainage system under Longlands field. It is intended that methods will be developed to apply the model to the whole of the catchment and other pesticides.

The model is driven by hourly rainfall taken from the automatic weather station (AWS), (Fig 1). The AWS also provides estimates of potential penman evaporation which have been taken as actual evaporations where the water content of the surface boxes is sufficient to meet the demand. The values of moisture volume fraction corresponding to SMIN, SMAX and SFC used in the model simulation are given in table 1. The values of SMIN and SMAX, with exception of Box 4, are based on PF curves generated for Longlands field by staff of the Agrohydrology section of the

Institute of Hydrology; values of SMAX for Box 4 were adjusted to allow the prediction of the onset of drain flow to match reality. The values of SFC are best guess estimates.

Table 1. Values of the moisture volume fraction equivalent to minimum water content (SMIN), field capacity (SFC) and saturation (SMAX), used in the model.

Box No.	SMIN	SFC	SMAX
1 and 5	0.19	0.27	0.49
2 and 6	0.24	0.32	0.40
3 and 7	0.30	0.35	0.38
4	0.24	0.25	0.31

The organic carbon content of the soils in each of the model boxes was estimated from analysis of soil profiles carried out by the Soil Survey and Land Research Centre. These values are given in Table 2.

Table 2. Organic carbon content allocated to the boxes used in the model.

Box No.	%Organic C
1 and 5	1.8
2 and 6	1.1
3 and 7	0.3
4	0.3

The application rate of isoproturon to Longlands was supplied by ADAS Rosemaund and is reported in section 3.2, table 1. The K_{oc} value used in the model is 130 and the degradation rate used was 1.44×10^{-3} hours^{-1}. The degradation rate is assumed to be the same in all boxes. No changes in degradation rate are currently made as a result of temperature, soil moisture content or depth.

Results and Discussion

The results presented here are from a very preliminary application of the model and should be viewed as a first attempt at using the model outlined above. The model was run using hourly data from 1 Sep. 1990 to the 31 Mar 1991 and output data were produced for the entire period. The results presented here are for short periods of time, coinciding with rainfall events, for which data on isoproturon concentrations were collected. Figures 3, 4 & 5 show simulated and observed values of drain flow and isoproturon concentration for the periods 8/9 Jan. 1991, 21/22 Feb 1991 and 4/5 Mar. 1991 respectively. For the last of these events no drain flow data are available.

Drainflow

Figure 4 shows that the model did a good job of simulating flows over this event. However the simulation shown in figure 3 is clearly less good. While the peaks of the hydrograph are simulated well temporally, the dynamic repose of the model is too slow for this particular event. This may be because this was the first drainage event of any significance. The drainage system was not working in the classic way at this point i.e. there was no 'gull winged' shaped water table above the drains (Bell *et al*, 1992). The soil above the drain was draining water rapidly down the profile and into the backfill and hence the drains. However, since there was no water table some of the drain water will leave the drain to recharge the ground water, while some will exit the drainage system. This will result in a very flashy response at the drainage outlet. Since the way the model is set up only allows water to exit the drain when there is a water table (i.e. in the classic drainage situation) then the model will do much better when this is the situation in the field. Therefore it should be expected to reflect reality better in the February event than in the January event, which it did.

Isoproturon

Figures 4 and 5 show that the model does not reflect any of the variability in isoproturon concentrations measured at the drain outfall, but does seem to agree well with the mean value about which these variations occur. There seems to be no obvious physical explanation for the variability in the measured concentrations and some of it must be attributable to expected error in the chemical analysis at such low concentrations. It is therefore reasonable to suggest that the model simulates these events quite well. The first event once again presents a problem with the estimated concentrations exceeding the measure values by more than a factor of 10. It is possible that this is linked to the problems noted with flow above. The model structure is such that the majority of the recharge to the bottom box is produced by the movement of a great deal of water through the high conductivity area above the drains. Consequently dissolved pesticide is transported fairly rapidly to depth and the concentration of the bottom box increases. In reality the water maybe moving rapidly in the larger pores which will not give it time to reach equilibrium concentrations with the surrounding soil. Further a proportion of water may not contact soil at all if it is moving down the middle of the larger pores. In either case this would result in a slower transference of pesticide to depth than predicted in the model.

Conclusions

The simple model of longlands field constructed on the basis of the process studies carried out has shown some promise. The simulation of isoproturon and flow in periods of classic drain flow are good. More work needs to be done to model the processes that control the transition period from no drain flow to classic drain flow which seem to exist in Longlands.

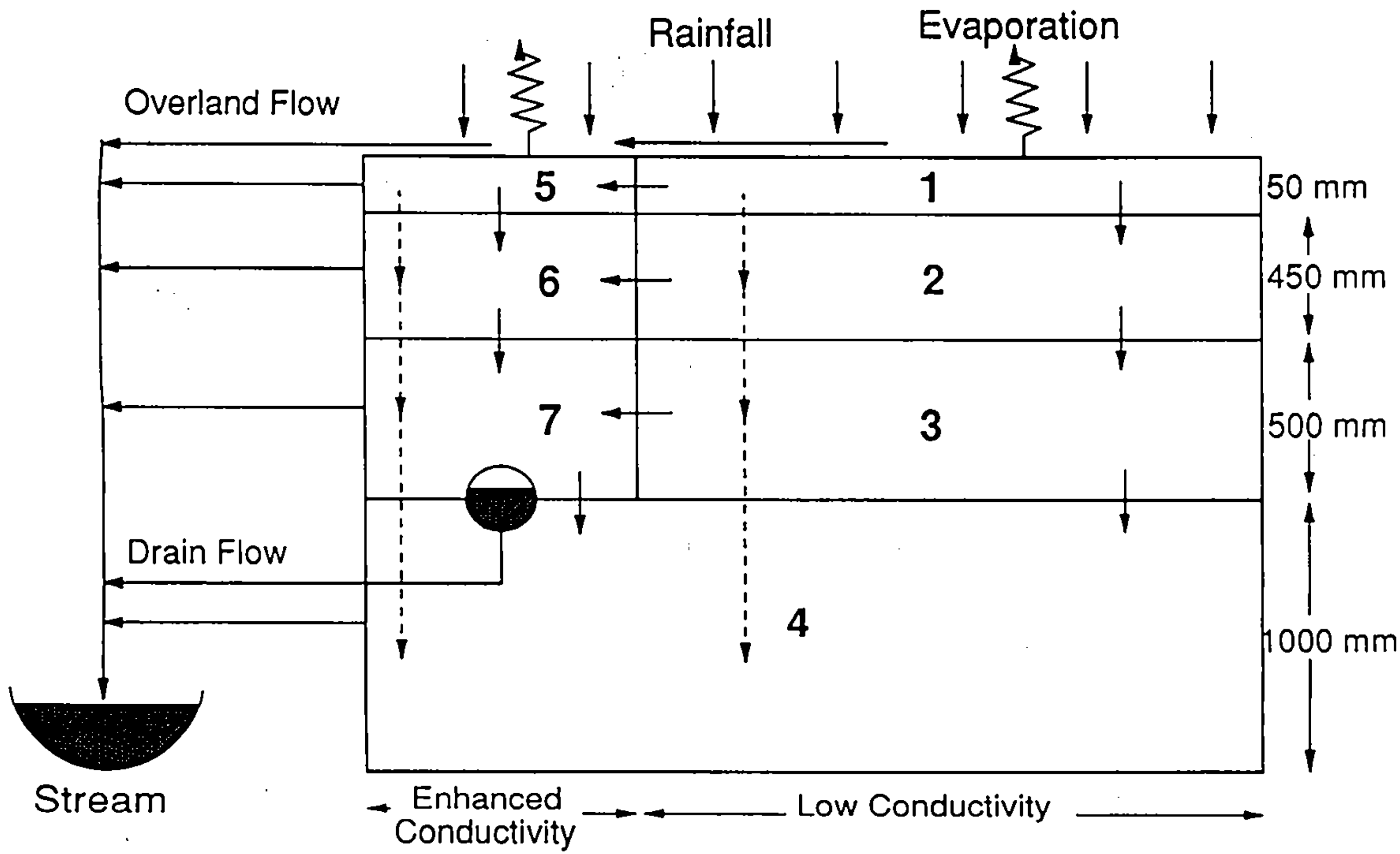


Figure 1 Schematic diagram of the Rosemaund pesticide model

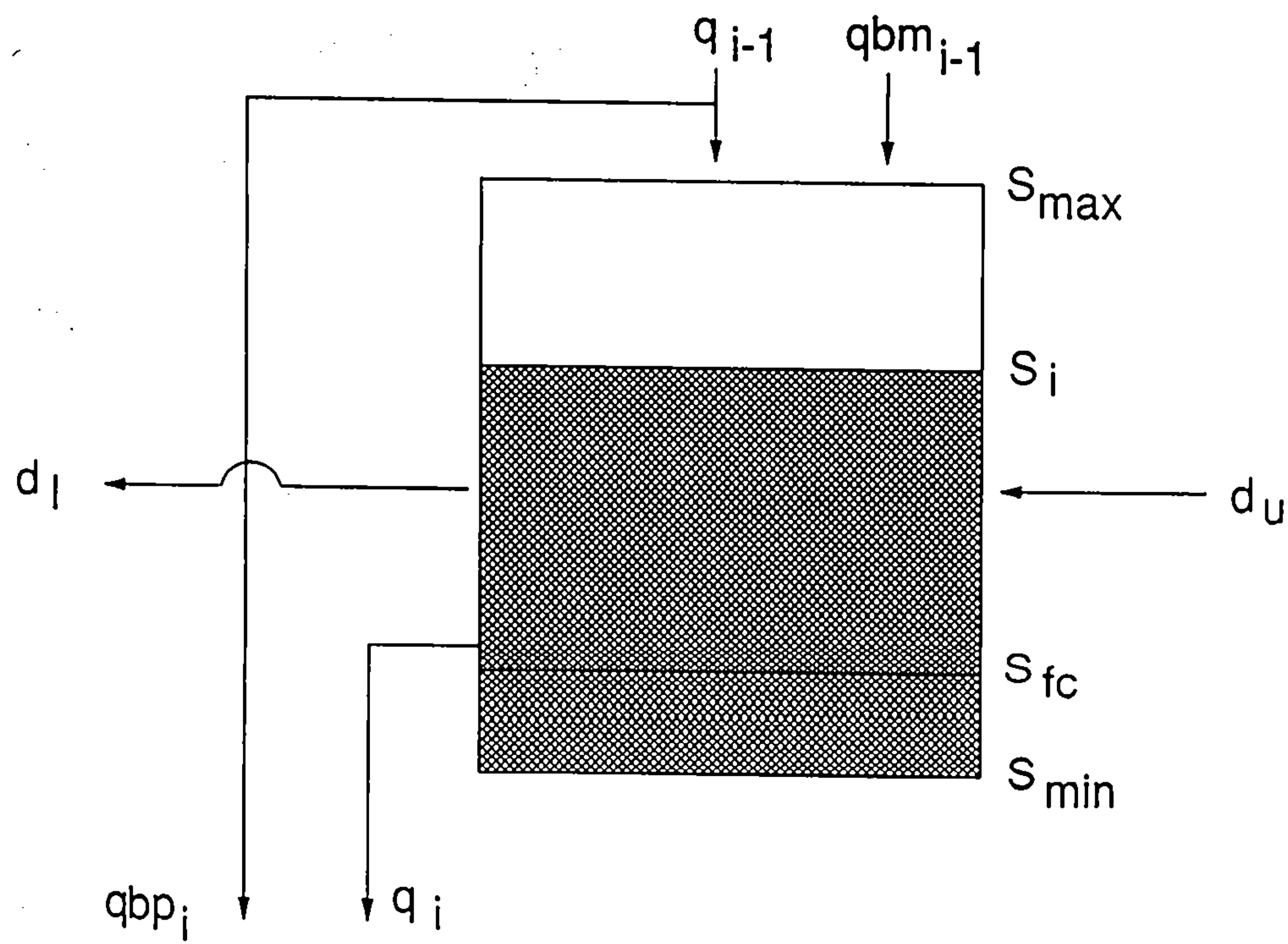


Figure 2 Details of flow through one box from the Rosemaund pesticide model

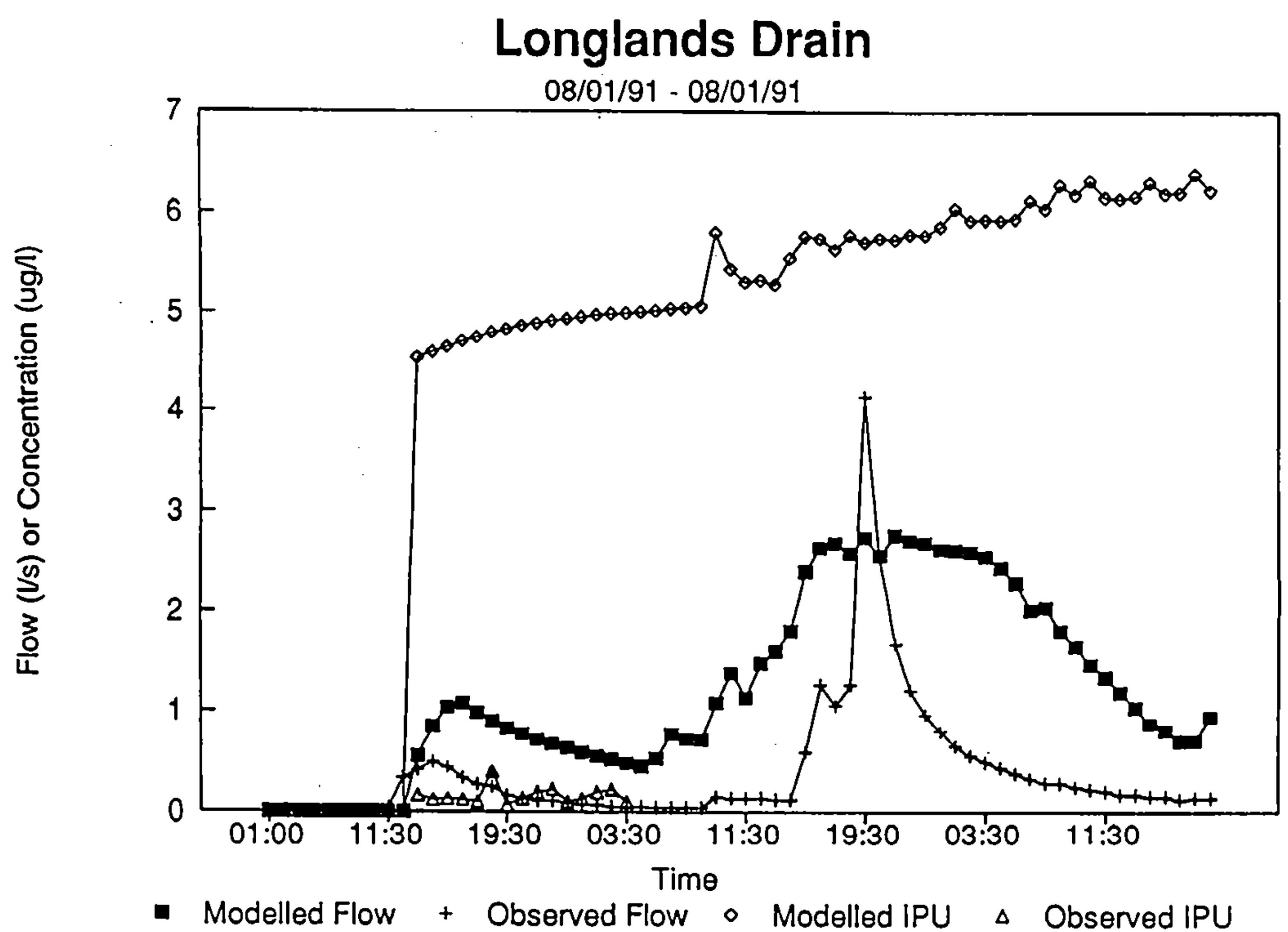


Fig 3 Modelled and observed flow and Isoproturon at the exit from Longlands Field drainage system

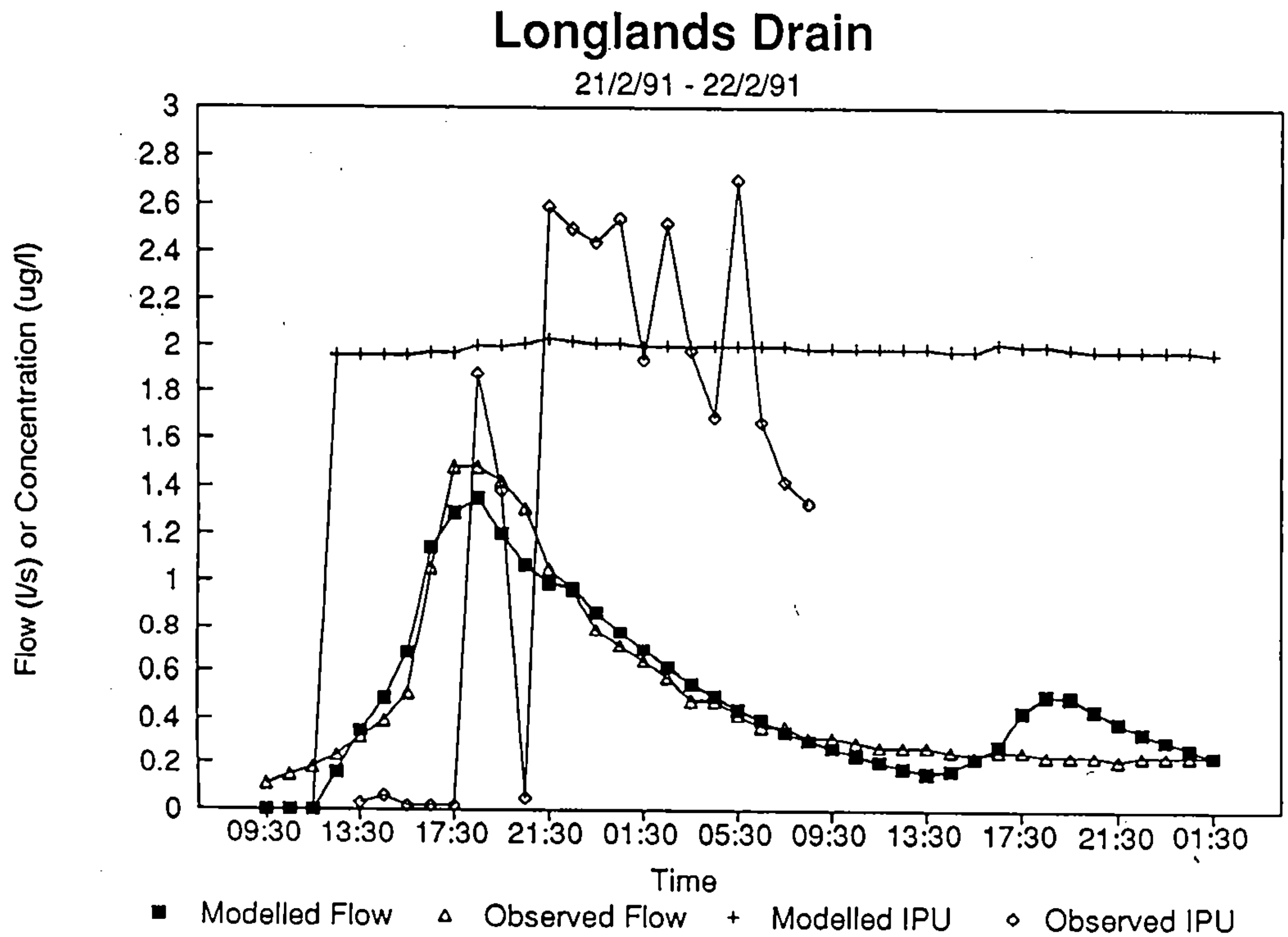


Fig 4 Modelled and observed flow and Isoproturon at the exit from Longlands Field drainage system

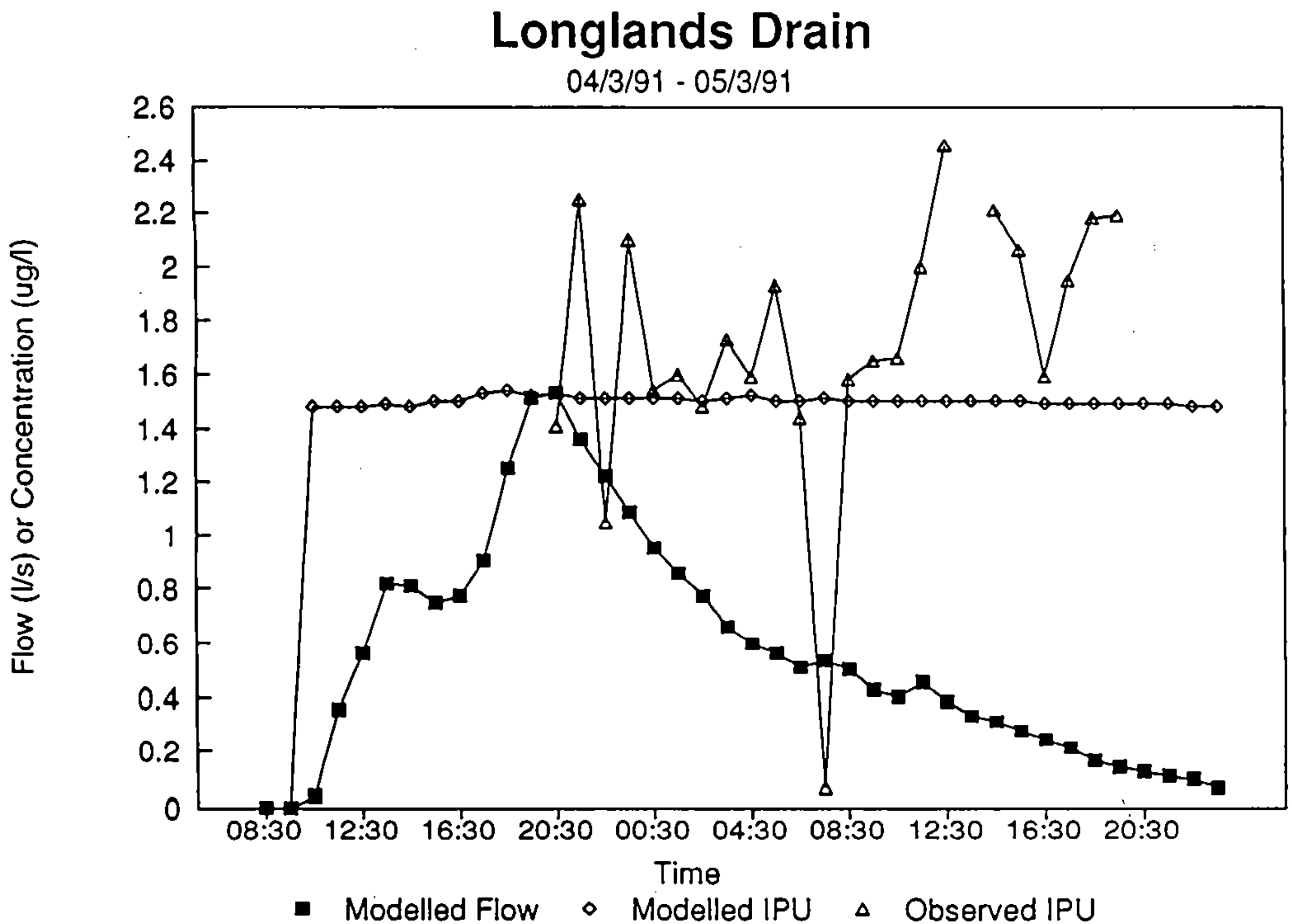


Fig 5 Modelled and observed flow and Isoproturon at the exit from Longlands Field drainage system

APPENDIX 9

DRAFT

PROPOSALS FOR THE IH LOIS DATA CENTRE

Document Number LOIS/IHDC/1a

9 July, 1992

Institute of Hydrology
Wallingford
Oxon
UK
OX10 8BB
Telephone (+44)(0)491-38800
Facsimile (+44)(0)491-32256

Abbreviations

GIS	Geographical information system
IH	Institute of Hydrology
IHDC	The IH Data Centre
LOIS	Land Ocean Interface Study
NERC	Natural Environment Research Council
NTF	National Transfer Format
WIS	Water Information System

Table of Contents

INTRODUCTION

This report has been prepared in response to a request from the Land Ocean Interface Study's Data Committee, made on the 1 July 1992. It outlines how a LOIS data centre could be set up at the Institute of Hydrology to serve the needs of river and coastal research within the LOIS programme.

PERCEIVED REQUIREMENT

Introduction

At the time of writing the LOIS project is still in the process of being defined. No research projects have been awarded. The requirements identified here are therefore based on:

- the LOIS Science plan
- informal conversations with members of LOIS committees
- some early assessments of the types and amounts of data likely to be involved
- IH experience of running the National Water Archives
- IH experience in the establishment and running of major archives in the former water authorities and the present National Rivers Authority

Perceived core requirements of the LOIS project

Data are seen as vital to the LOIS project.

It is thought that the assembly of large high quality data sets in an easily accessible form will make many new avenues of research possible.

It will be a condition of receiving LOIS money, that researchers will send their data to nominated data centres immediately after collection and that they make their data available to other researchers. NERC data policy will apply.

Researchers will be responsible for the quality and documentation of their data.

There is therefore a requirement for one or more appropriate data centres to be established for receiving, auditing, storing and disseminating data.

Given the time frame, it would be infeasible to create a single data centre capable of supporting all the diverse requirements of likely LOIS researchers without striping NERC

Institutes of essential staff. It would also require significant accommodation and have large setting up costs with respect to equipment. It therefore seems more practical to build on existing facilities and improve the links between those facilities and between those facilities and their users.

If that is accepted and given that the objective of LOIS is to study the interface between the land and the ocean, there will be important requirements to:

- exchange data between data centres easily
- ensure common definitions of data
- define standards for data
- establish quality control procedures
- establish quality assurance procedures including auditing

For river and coastal studies, there will be a requirement for a database capable of handling spatially referenced time-series data. It is currently assumed that this role will be filled by the Institute of Hydrology's system WIS.

This database will hold both core data and data arising from thematic studies. The possible data sets are elaborated below.

Perceived requirements of LOIS thematic studies

It follows that if researchers have to submit their data to the data centres, then the data centres must be staffed and equipped to receive and load data immediately.

If LOIS researchers are to obtain any benefit from having to submit their data to a data centre, then they will require much more of the data centre than simply being a safe repository. They will also expect it to provide the tools for analysing their data. Because the data volumes can be very large, analysis packages are often inextricably linked to the database that holds the data. The analysis package will need the data structures of the database in order to be able to manipulate the data.

Therefore LOIS users will at the very least require the data centres to provide simple analytical tools for the examination of data and could reasonably expect to find much more than just the basics.

Data cataloguing facilities will be essential.

LOIS researchers will also require documentation, training and support in the use of facilities provided by the data centres.

The data centres will not be able to provide every analytical facility that researchers will require. It would be quite reasonable for them to expect to be provided either with direct on-line access to the storage system or with a copy of the storage system which they could mount on their own machine. Either way might enable them to interface their models and applications directly to the database. It could also facilitate data transfers.

It would seem reasonable that LOIS researchers who do not have access to work stations and similar equipment should be able to visit the data centre and avail themselves of the facilities there.

PROPOSED FACILITIES

Introduction

The facilities outlined below are designed to meet the requirements identified above. For the purposes of estimating, the task has been assumed to be comparable to running a database for a region of the NRA. There will be a large up front setting up task, which will take place over the first year, which the NRA would not ordinarily have, however, this is probably offset by LOIS having a lower rate of data acquisition. An NRA regional team would typically be staffed by 6 or more people. Two and a half people are proposed here, as some of the activities would be carried out by IH anyway.

Services

IH will provide the following services to users of the data centre:

set up the Water Information System

define and maintain data standards in collaboration with other LOIS data centres

define and maintain a data model for river and coastal data

agree data inter-change procedures with other LOIS data centres

set up and maintain core data sets

register LOIS researchers

provide advice to LOIS researchers

receive LOIS researchers data

audit the supply of researchers data

provide access to data

provide limited facilities for visiting LOIS scientists

Computing

Hardware

The Institute will provide the hardware to support the IHDC.

Software

The Institute will provide the Water Information System to the IHDC.

The Institute will make the Water Information System available free of charge to LOIS researchers for use on their own hardware for work in connection with LOIS. The researcher will be responsible for any training, maintenance, support and documentation costs though the Institute will endeavour to keep these as low as possible.

Communications

It is unclear what is required here at present, but it may be that some inter-organisation communications will require upgrading, if WIS systems are to be used for on-line remote access the IHDC database.

Data

Core data

The Institute will make available (SOLELY FOR LOIS RESEARCH):

the IH DTM (through our framework agreement with OS)

the IH digitised river network

the Flood Studies Report maps

Subject to discussion and NRA agreement, IH could acquire NRA water quality data in the public domain.

Subject to agreement within and without IH, which it has not been possible to obtain within the time frame for preparing this report, it may be possible to make other data sets available, such as:

soils related data

data on artificial influences on river flows the National Water Archive records of river flow

ground water data

lithological logs

meteorological data

land use data

LOIS researchers will be responsible for respecting any copyright conditions associated with data made available by the IHDC.

Data from thematic studies

The acquisition of additional data for thematic studies will be the responsibility of the researcher.

METHOD OF OPERATION

At the start of a LOIS research project the researcher will register as an IHDC user.

The researcher will define his requirements for data storage and retrieval. If this requires facilities beyond those available, the researcher will be responsible for the cost of extension.

The researcher will agree with IHDC a program for delivery of any data to the IHDC.

The researcher will agree with IHDC a data model for the storage of any data, using where feasible the standard IH data model.

The researcher will be responsible for the timely delivery of data in an agreed format, likely to be NTF.

The researcher will be responsible for the quality control of delivered data. Any quality control software or algorithms employed will be made available to IHDC if appropriate so that a library of quality control software can be established.

The researcher will be responsible for ensuring that delivered data are adequately internally documented so that subsequent users can ascertain their fitness for other purposes.

On receipt of researchers' data, IHDC will:

log their receipt

pass the data through IHDC's quality control procedures notify the user of rejected or suspect data

load data that pass the procedures onto the archive

Researchers will be able to access data in the following ways:

by visiting IH by prior appointment and using IHDC's facilities

by written/E-mail request

by remote access - method to be defined

by remote access using WIS

SUPPORTING R & D

A highly beneficial outcome of projects such as LOIS is that they lead to demands for new types of facility. A small part if the IHDC's effort will be directed towards the monitoring of these demands and the research and development necessary to produce solutions.

RESOURCES

Staff

It is proposed to staff the IHDC as follows:

LOIS rivers and coastal database manager	(SSO)
Scientific support	(HSO)
Archivist	(1/2SO)

Equipment

The following equipment will be required:

Advanced graphics work station	1
Personal computers	2
Server	1
Communications enhancements	
Software for the above e.g.	
Oracle	
Fortran	
C	
Word processor	
etc	

Accommodation

Offices for IHDC	2
Office for visiting scientists	1
Storage rooms	1

IMPLEMENTATION PLAN

The implementation plan for the IHDC will follow the guidelines set out in the WIS outline implementation plan.

COST

Costs are estimated as follows:

Capital	£120,000
Recurrent	£125,000/year

N.B. These are preliminary costs and will need to be confirmed when clearer requirements have been defined. Provision for hardware and software maintenance costs are not included as these are not currently known. As a guide, it is believed that NCS are likely to charge £4k/year per work station and £400/year per PC.

N.B. Additional to any base-line funding.

APPENDIX 10

COMPUTING PROVISION for LOIS

Contents

1. Background

Important aims of LOIS include initiation of "the development of coupled land-ocean models of environmental change in the coastal zone" and, as part of this, to develop the use of GIS in the handling of spatial data sets, visualisation and interfacing to numerical models. These activities are potentially demanding of computer facilities (processing power, data storage and retrieval) beyond the capacity of individual workstations.

2. Objectives requiring computers

2a. Models

RACS(R) (management by IH; location at IH and universities)

- to predict fluxes of water, sediments etc. leaving catchments for rivers and the coast/estuary, for different scenarios of climate and land use; 3-D catchment/soil models calculating water flux and nutrients, pesticides, organics, metals and sediments, applied to large catchments over time-scales of land-use change and climate change;
- river flow and quality models to calculate flows and contaminant loads for river/estuarine boundaries, including the North Sea Project period.
- groundwater models will be required to compute flow and quality fluxes interacting with coastal ecosystems, rivers and catchments.

RACS(A) (management by UEA; location at UEA and Liverpool?)

- calculation of air-mass properties (constituents) along back-trajectories.
- numerical simulations to evaluate the significance of atmospheric processes on coastal-zone budgets.

RACS(C) (management by PML; location at PML and POL with collaboration from IH and universities)

- estuarine modelling: 2- and 3-D models of the Humber estuary, which can accept realistic inputs from catchment and coastal sea models; sediment and solute transport will be modelled; the role of the estuary in storing and releasing sediments will be investigated for a range of scenarios;
- coastal strip modelling: fine-resolution 2-D and 3-D hydrodynamic, solute and sediment transprot models for the coastal strip between the Tweed and the Yar; the models will be used for interpretation of physical, chemical and sediment observations, as a dynamic background for process models of chemistry and biology, and for investigating historical scenarios;
- chemical/biological modelling: development by combining conceptual models of

chemical interactions (involving solutes, suspended particles, bed exchange and biological uptake) with coastal-strip and estuarine hydrodynamics, to investigate and improve the models; the models will be tested against data collected on the RACS cruises;

- ecosystem modelling: a North Sea ecosystem model will be adapted to the RACS coastal region, to lead towards a coastal carbon flux model.

SES (management by UCNW and POL; location at POL with collaboration from DML, IOSDL, PML and universities)

- eventually, to integrate up from process studies to estimate total cross-slope exchanges and budgets;
- shelf-edge prognostic, 3-D with 1 km resolution, to be implemented in 56-57°N × 8½-10½°W within a shelf model, and developed to incorporate transports and source-sink terms for sediments, constituents and biological variables; verification including comparison with simpler models; sensitivity-analysis runs for significance of various processes; flux estimation;
- data assimilation methods; data visualisation;
- matching a shelf model to an ocean model.

LOEPS/NORMS (management by University of Cambridge and BGS; location at BGS, POL and universities)

- to model the changing tides, patterns of shelf-sea stirring, sediment transport paths and hence evolution of the shelf system in response to Holocene changes in sea-level and glacial rebound. This involves extended runs of a shelf-wide model with sediment transport and speeded-up bed evolution; see also *NORMS geomorphology*.

NORMS (management by POL; location at POL, PML, IH, BGS and universities)

- water-quality models, shelf-wide with appropriate land and ocean boundary conditions, embodying hydrodynamics and non-conservative constituent behaviour; specific example constituents to include a nutrient, trace metal, a land-ocean flux tracer and an organic pollutant. These will be developed *via* a 3-D 2½ km hydrodynamic model from the Dover Strait to 56°N, accepting freshwater inflows and surface heating; extension shelf-wide accepting ocean boundary conditions; development to incorporate transports and source-sink terms for constituents; extended runs (months-years; specifically the 15-month North Sea Project period) with feasible resolution. A corollary is to construct shelf-sea budgets with the shelf-wide models as an integration of RACS and SES. (At POL).
- geomorphology: models addressing decade-to-centuries evolution with a coastal focus[1] (extending offshore as far as the involved sediment transport, and alongshore from eg. Flamborough Head to Norfolk) assessing the impacts of sea level, storm frequency, rainfall, freshwater, land use, ... through scenarios spanning the past eras of measurements, documentation and post-glacial records. Catchment/river inputs[2] and shelf-sea scenarios of wave/tide/surge[1] will be off-line boundary inputs from model runs. Development of wave (WAM model) interactions[3] forms an important part of this study; ecosystem model feedback is anticipated later. (Calculations at [1]POL, [2]IH, [3]POL & universities).
- buffering of fluxes of the same water quality variables received from catchments from the Tweed to the Wash, in the estuaries and a coastal strip[1] including the interacting outflow plumes (eg. Humber-Wash; a RACS objective), to be modelled for a range of scenarios representing changed conditions over the last 200 years (the specific NORMS aspect). This may involve developing parametrisations for the extended runs (months-years) required to assess the relative contribution of "events". Catchment/river inputs[2] and shelf-sea tide/surge[3] scenarios will be off-line boundary inputs from model runs. (Calculations at

[1]PML+POL, [2]IH, [3]POL).

- later carbon cycle (ecosystem) models for community structure and function, with nearshore, terrestrial/riverine, atmospheric and geomorphological model input. Contexts are the marine water column and possibly dunes, eroding cliffs, saltmarsh, mudflats, offshore banks... according to systems studied in RACS(C). Questions may be eg. *What is the impact of land-derived nutrients on the offshore ecosystem?* and *Given the rate of sea level rise, what is the rate of spread of X?*

- the development of management tools, subject to commissions from responsible authorities.

2b. DATA

(management by, and location at NUTIS and the data centres BGS, IH, ITE, BODC, with collaboration from universities)

- rivers data base at basic 1 km resolution (soil, land use,..) and in some respects finer (30-50m: topographic contours, catchment boundaries; land use in selected catchments from LANDSAT); the Water Information System (WIS) for LOIS will store all hydrological and chemical data compiled for LOIS catchments and rivers as well as information on digitised river networks;

- GIS database for coastal zone, including standardised coastline and high-resolution bathymetry;

- smooth data transfer between ship and shore (as North Sea Project and BOFS)

- GIS → three dimensions and time, to combine different dimensions (eg. OSCR + ADCP, AVHRR + CTD), to develop efficient storage (or multi-dimensional relational database, eg. ORACLE as used by BODC);

- incorporation of statistics, eg. correlations, in GIS;

- study of error propagation in GIS;

- study of data visualisation techniques (including standardised handling of remote-sensed data, and model output);

(To be financed by the respective LOIS components)

- processing and quality control of the diverse marine data collected during SES and RACS and their assembly into coherent data sets (BODC).

- RACS(R) data centre.

- LOEPS data centre, developing GIS (part-financed by *Data*?), modelling surfaces, displaying interpreted seismic sections, etc. (BGS).

- LOIS ecological data centre, especially land cover (also soils, climate, topography ...) and design to allow integration of field observations therein (ITE Monks Wood).

- assembly of ancillary and historical data sets;

- production of accessible on-line databases, then off-line data-base products, eg. CD-ROMs;

- final archiving of data.

3. **Detailed Computing Needs**

3.1 *Development paths*

(by years in LOIS; year 1 = 1992/93) Table 1

Model\year	1	2	3	4	5
catchment	3D sub-catchment flow	reduced-order plane model and sediments	sediment metals nutrients	land-use scenarios	alternative climates
rivers	1D & 2D	sediments chemistry	biology	generalised sensitivity analysis	scenarios
groundwater	2D & 3D catchments	coastal zones	chemistry	land use scenarios	climate scenarios
coastal	estuary, esp. sed.transpt (1D exists)	coastal strip scenarios	chem & bio sediments metals	partitioning plankton-uptake	ecosystem
shelf edge	develop on wksta.	overflow to supercomp.	expand area nest in shelf	ocean/shelf	ocean circ. coupled
palaeotides	link wave & tide/surge	---- develop 2D wave/ tide/surge	sed. transpt 10 runs shelf@12km		
water qual. to 56°N	physics (exists)	2½km -----	water qual.	--------------	
water qual. shelf-wide			---- ~2½ km physics ----	- 20 levels - water qual.	48-63°N, 12°W-10°E +shelf edge
estuarine buffering	(uses river/ catchment & coastal)	10 cases - steady wind - 2D coastal	-------- strip - 3D -	10 scenarios 400×50km	----------- @ 1km × 50 levels
coastal geomorph.	link wave & 2-D tide/surge	develop 3D	& sed.trnspt ------------- 2D wave/ tide/surge	10 scenarios 400×50km @ 1 km	----------- 3-D with 50 levels

Catchment and river models have been run for fine-resolution 3-D simulations on the RAL Cray XMP. Development work is difficult because of slow turn-round. However, production runs of full LOIS models will demand major facilities which cannot be met by LOIS machines.

Marine models with fine resolution (nearshore or frontal), shelf-wide 3-D current models and wave models, and fine-resolution shelf-edge models, have been run on the RAL Cray XMP for some years, owing to their large computing requirement. At present, some transfer of development work to local workstations is taking place, enabled by rapidly increasing processing power thereon, and motivated by convenience. However, "production runs" will continue to demand the largest facilities available, as in the case of entries in the *Supercomputing* tables 4, 5 below which cannot be met by a LOIS machine.

3.2 *Database needs*

Several present data bases for river catchments are at 1 km resolution (soil, land use) or finer (30-50m: topographic contours, catchment boundaries; land use in selected catchments from LANDSAT). For a modest area, a Silicon Graphics will run the Water Information System (WIS) faster than the Wallingford IBM. The Plynlimmon area (Severn & Wye headwater catchments) is 4 Mbytes; an estimate for WIS in LOIS is 20 Gbytes.

For data storage and GIS development, NUTIS already utilise a Meiko computing surface with an 8 × T800 transputer array.

(The following are candidates for finance by the respective LOIS components).

Most of the oceanographic data will be processed and quality-controlled using BODC software systems running on Silicon Graphics workstations - the data being stored and managed on optical discs as part of a mass data store at POL (baseline funding).

The RACS(R) data centre will want a server (IH).

The LOEPS data centre needs a workstation (~ £30K) and software (BGS, LOIS→ES top-sliced funding).

The ecological data centre wants a workstation and Laserscan HORIZON licence.

3.3 *Remote sensing*

An interest in image-processing software has been identified (for the ecological data centre) which should be in common with other LOIS interests in visualising data and model output.

3.4 *Consequences of not meeting these needs*

There would be severe delay in developing shelf-edge models with stratification and bathymetry with the fine resolution which this context demands.

Shelf-wide density-evolving models could only run on the RAL YMP. The largest model run with practical success on a workstation (HP 9000 model 730 running at ~20 Mflops) has ~1000 horizontal grid points (20 km resolution from Dover Strait to 56°N) × 20 vertical; it takes 12 hours to run 2 simulated months.

Similarly, the IH catchment model, simulating a single slope (x,z) using

240 finite elements × 500 time steps for 20 days × 4 iterations per step

uses 2 Mflops hours (ie. 1 hour per simulated month) on a Silicon Graphics Indigo. It would be difficult to develop this to 3D on a workstation.

Dedicated LOIS use and control for rapid turnaround and data transfer is part of the case. Sharing and especially contracting out are therefore inappropriate. Leasing *vs* purchase may be regarded as a purely financial decision.

Scaling down is directly reflected in limitations on the realism (resolution and processes included) of the models that can be developed. They have firm requirements of processing speed (Mflops) and on-line memory related to model size and number of computational cycles.

Various configurations of off-line data storage and disk space might be considered. For the scientific objectives of LOIS, it is considered that the connection between catchment/river and marine models can be off-line.

Coupling of workstations may result in a system which is communications-bound for environmental models characterised by many repetitive calculations on large arrays whose values interact. This is not a primary solution for LOIS, pending further development.

4. Computing considerations and options

Three ranges of computers are considered:

- individual PC/workstation systems costing about £20K or less. (At present, this corresponds to about 20 Mflops or less, and disk capacity to a few Gb; however, the top end of this range is changing rapidly);
- a National Centre, especially the RAL Cray Y-MP, prospectively enabling processing at up to about 2 Gflops;
- "in between" these, entry-level supercomputers or "computing engines", up to 1 Gflops, and prospectively dedicated to LOIS.

4.1 *Individual PC/workstation systems*

Many computing needs will be satisfied by these. It is envisaged that they may be purchased as part of Special Topic awards or home laboratory provision, as necessary and appropriate. The principal consideration is that compatible operating systems (probably Unix) will facilitate the linkage of different models. Similarly, there is an advantage to common means of visualising remote-sensed and model-output data. These considerations, and favourable terms, argue in favour of a bulk purchase of such smaller systems at the time of Special Topic awards.

Estimated numbers required for modelling projects are shown in the following tables; others will be needed for data processing, etc. Here C - "number-cruncher" (eg. 6Gb disk, 32 Mb memory for the PML group estuarine, coastal, ...), G - graphics, W - "low-end".

Component-funded (workstations, etc.) *POL, PML et al.* Table 2

Model\year	1	2	3	4	5
estuarine coastal strip chemical/biology ecosystem ECoS....(all PML)	1C 1/4G 1C 1/4G PC + etc.	@ 1-p-1 @ 1-p-1 1C 1/4G 1C 1/4G @ 2-p-2	------------ ------------ @ 1-p-1 @ 1-p-1 ------------	------------ ------------ ------------ ------------ ------------	------------ ------------ ------------ ------------ ------------
shelf edge	1C 1W	3C 2G 1W	3C 2G 1W	3C 2G 1W	3C 2G 1W
palaeotides		1C 1G	1C 1G		
water qual. to 56°N	1C	2C 1G	1C 1G	1C 1G	
water qual. shelf-wide			1C 1G	1C 1G	2C 2G
estuarine buffering		2C 2G 1W	2C 2G 1W	2C 2G 1W	
coastal geomorph			1C 1G	1C 1G	1C 1G
Total	4C ½G 1W	12C 7G 2W	13C 9G 2W	12C 8G 2W	10C 6G 1W
purchase		8C 6½G 1W	1C 2G		

Component-funded (workstations, etc.) *IH et al.* Table 3

Model\year	1	2	3	4	5
catchments	1C 1G 1W	2C 2G 1W	2C 2G 1W	2C 2G 1W	2C 2G 1W
rivers		1C 1G 1W	1C 2G 1W	1C 2G 1W	1C 2G 1W
groundwater	1C 1G 1W	1C 1G 1W	1C 2G 1W	1C 2G 1W	2C 1G 1W
Total	2C 2G 2W	4C 4G 3W	4C 6G 3W	4C 6G 3W	5C 5G 3W
purchase		2C 2G 1W	2G		1C

It is also expected to carry out all RACS(A) modelling on laboratory- or RACS(A)-funded workstations or smaller.

4.2 *National Centre*

The very largest models should be run thus.

From a national viewpoint, the cost of running jobs at a National Centre, rather than on LOIS machines, should be taken into account. Estimates for costs of a unit calculation are

	Cray Y-MP 8 cpus	Cray YMP EL 4 cpus	Cray YMP EL 1 cpu	work-station
capital cost	5.2 M	500 K	200 K	20 K
per annum over 5 years	1.04 M	100 K	40 K	4 K
plus 10% maintenance	1.3 M	110 K	44 K	4.4 K
utilisation	70%	50%	50%	10%
cost per hour	400 (8 proc)	25	10	5
sustainable Mflops	1500	320	80	10
hrs for 100 Mflops.day	1.6	7.5	30	240
cost for 100 Mflops.day	640	188	300	1200

Thus it is appropriate to run *only* the very largest models at a National Centre, so that they have full scope, and so that supercomputer performance is not degraded by scheduling many jobs. To some extent, this is also a LOIS viewpoint, some LOIS jobs eventually being among these very largest.

4.3 *Dedicated LOIS machines*

Hence this report is concerned with needs for rapid data transfers beyond a few Gb, individual needs for large on-line memory, calculations requiring tens to hundreds of Mflops, and hence especially the case for a powerful "computing engines", up to 1 Gflops.

From the specific viewpoint of LOIS, a two dedicated machines are essential to ensure: access for rapid turnaround and visualisation during model development; project control to guarantee the turnaround; high levels of intra-project interaction through the use of common computing and transfer media, visualisation packages and visits to the site by the several LOIS user groups. Both POL and IH have removed some models from the RAL Cray XMP to in-house workstations (where feasible) to obtain the turnaround and rapid visualisation needed for development. It should be noted that at POL this is *despite* the presence of six "original" users of the Cray 1S at Daresbury.

Such machines should be at a well-networked site, to aid remote access and encourage joint work by LOIS scientists at different locations. To minimise network traffic (another argument against use of a National Centre) they should be where most computing is generated. The status of super-JANET with data transfer rates O(0.1 GB / sec) is uncertain at present. However, it may be assumed that O(2 Mbit/sec or 5 Gbit/hour) transfers will be possible to IH and POL through relatively short links to the JANET trunk lines. This rate (roughly one screen image per second) is marginal for data transfer and visualisation, but quite inadequate for video.

Any chosen systems will need to run within a Unix network.

Any chosen systems needs to be "downward compatible" to run and link models initially developed on workstations, and "upward compatible" for eventual transfer of uprated models to an upgraded system and eventually a National Centre.

The need derives from entries in the following *Supercomputing* tables. They show the number of people involved (individuals-p-**full time equivalent**); computing need in days @ 100 Mflops; in/output data volume (on-line = **memory in MW**, off-line = ***storage in GB***)

Supercomputing, POL Table 4

Model\year	1	2	3	4	5
shelf edge lim. area nest in shelf ... in ocean	2-p-1½	6-p-4 40 6 *10* 60 24 *100*	6-p-4 70 24 *100* 150 24 *200* (National	6-p-4 40 24 *25* 200 48 *200* centre) ---	6-p-4 250 48 *200* 2000 200 *2000*
palaeotides		6-p-1 1 90 *3*	6-p-1 2 90 *7*		
water qual. to 56°N	3-p-2 10 30 *100*	4-p-3 30 30 *250*	2-p-2 40 60 *200*	2-p-1 40 60 *200*	
water qual. shelf-wide			2-p-1 50 200 *400*	2-p-2 100 200 *800* (subset)/	3-p-2 100 200 *800* (subset)/
estuarine buffering		4-p-3	4-p-3 3 50 *10*	4-p-3 5 50 *20*	4-p-3 5 50 *20*
coastal geomorph			6-p-2 5 100 *10*	6-p-2 12 100 *25*	6-p-2 12 50 *25*
Totals	p-3½	p-11	p-13	p-12	p-11
plus	10 30 *100*	131 90 *363*	270 100 *527* 50 200 *400*	297 100 *470* 100 200 *800*	267 50 *445* 100 200 *800*

Supercomputing, IH Table 5

Model\year	1	2	3	4	5
catchment		4-p-3 150 100 *200*	4-p-3 200 100 *200* Natn'l Centre	4-p-3 250 100 *200* 2K 200 *1K*	4-p-3 250 100 *200* 2K 200 *1K*
river		2-p-2 30 50 *100*	2-p-2 40 50 *100*	2-p-2 100 50 *100*	2-p-2 100 50 *100*
groundwater		2-p-2 30 50 *100*	2-p-2 50 75 *100*	2-p-2 100 75 *100*	2-p-2 100 75 *100*
Totals		p-7	p-7	p-7	p-7
+ Ntn'l centre		210 100 *400*	290 100 *400*	450 100 *400*	450 100 *400*

4.4 *Software considerations*

Much present <u>code</u> is in Fortran-77; efficient compiled code is wanted from this, or translation effort to Fortran-90 which may become standard for super-computing. The more parallel the computer, in general the more specialist programming is required to exploit it effectively.

LOIS involves the interfacing of programs written by several scientists, and possibly used by others eventually. Appropriate structuring needs to be planned, invoking as appropriate design tools (eg. CASE), frameworks (eg. MAST-0050-C) and the experience of institute scientists. These structural aspects, and "user-friendly" "shells" for subsequent model applications (which should be funded by commissions), may benefit from professional programming assistance. (By contrast, process "modules" depend on scientific understanding and often the numerical and process aspects are intrinsically inseparable).

4.5 *Fast links*

The fastest links will be needed with the on-line memory specified in the *Supercomputing* tables. Fast channels will be required for visualisation and to accept the output of a fast processor (faster than FDDI) which will have to be served by closely coupled disks. For the large output volumes (see *Supercomputing* table), a mass store is required, at the same site; otherwise, Super-JANET. POL expects to have a mass store in early 1993; a workstation and large store at IH for I/O bound work (generated by *DATA* and WIS) forms one of the recommendations herein.

The O(2 Mbit/sec or 5 Gbit/hour) transfers possible through links to the JANET trunk lines, required for data transfer and visualisation, will need to extend to remote users of a LOIS machine (see §2a).

4.6 *In-house support*

To obtain the best performance from two LOIS dedicated supercomputers, a supercomputer specialist should be located at each installation site to advise and assist LOIS users. A sensible allocation of consumables should be assured, as well as reliable power supply and communications.

NCS at present support UNIX workstations at NERC sites.

4.7 *Hardware options*

For I/O bound work with large data storage rather than processing power requirements (NUTIS, WIS), a workstation may be appropriate, running with ~20 disks (and/or optical disks) of 1-2 GB each. Silicon Graphics and Intel have such systems. Cost: ~ £80K.

CHEST are negotiating to buy (by early 1993) a "package" for remote-sensed and aircraft data, eg. PCI EASI-PACE which links with PVWAVE and some existing GIS systems.

For supercomputers, the specification should include a machine's own fast disks. NCS (1992) have carried out test runs on the following machines.

Table 6

Machine	memory Gbytes	disk Gbytes	Mflops peak	Mflops achieve	£K	comment
SunSparc 10/54			80			
Cray EL 1-4 CPUs	¼-1	scope to expand	133-530	106-320	200-500	up/down compatible 4cpu max
Convex C3440	½		800	320 (32-bit:x2)	800	up/down compatible poor mem bw.
Intel iPSC/860	1		5120	500,(@ 32-bit)	800	special programs
KSR-1 32-proc	1	10	1280	320	730	reliability ?
CM-5	1	16	4000	400	750	special programs

Translation from the functional requirement to a choice of systems should also involve "user" experience, and benchmark runs of catchment and marine models for proper comparison between computers of different architecture. POLMP has already been widely used as a benchmark code which can be used as part of the procurement exercise. The IH Distributed Model has been used to perform the same task for catchments.

Value for money of available hardware has been increasing rapidly and may be expected to continue so doing. Hence the best value will obtained by purchasing just when the demand arises. It might also argue for a phased purchase, in which case the systems should be expansible.

Decommissioning of present NERC IBM mainframes will make space available.

Buying two smaller systems (rather than one larger) implies more expenditure on "metalwork" at the expense of total processing power, memory and disk. However, two machines will serve the two principal modelling communities at POL and Wallingford more efficiently.

5. Recommendations

- "Ordinary" workstations should be bought in bulk for maximal compatibility across LOIS, and for value for money.

- The use of common transfer media and visualisation "packages" should also be sought. It may be appropriate to tender before deciding. CHEST may settle the visualisation choice.

- There should be consideration of support for IT / program structuring.

- Some LOIS "production" runs will clearly need a substantial part of the provision at the National Centre, which should be involved in the planning.

- Visualisation and database interaction constitute an early demand for a workstation with O(20-40 GB) attached disks at Wallingford.

- The need for computer provision O(½ Gflops) at Wallingford and POL is clear, particularly to meet the needs of RACS(R), SES and NORMS model development. Purchase should be timed to coincide with overflow from workstation capacity, so that value for money is maximised as prices fall. This point may be expected in mid-1993, but is already the case for the southern North Sea model (due to memory needed).

- The *considerations* of networking (via JANET and to a mass-store and means of visualisation), down- and up-compatibility, compilation of existing code and benchmark testing should be respected. Scope for later addition of more processors would be an advantage.

Reference

NCS (1992) Introduction to computer modelling for NERC scientists. Report from the NCS computer modelling advisory group, version 1.0, May 1992, 41pp.