WATER FRAMEWORK DIRECTIVE –
The Application of Mathematical Models as Decision-Support Tools
(2002-W-DS-11)

TABLE OF CONTENTS

Environmental RTDI Programme 2000–2006

WATER FRAMEWORK DIRECTIVE – An Assessment of Mathematical Modelling in its Implementation in Ireland (2002-W-DS-11)

Synthesis Report

Prepared for the Environmental Protection Agency

by

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Synthesis Report Table of Contents

1 Introduction

EC Directive 2000/60/EC establishing a framework for Community action in the field of water policy, commonly known as the Water Framework Directive (WFD), aims to prevent further deterioration and to protect and enhance the status of aquatic ecosystems throughout the European Member States by 2015. The WFD needs to classify waterbodies based on assessment of ecological elements, including the hydromorphological and chemical conditions that support those elements, and, for groundwaters, quantitative and chemical status of the waterbody. The realisation of the demands of the WFD requires development and implementation of a number of technical tasks that relate to characterisation of catchments, monitoring procedures, establishing the relationship between catchment pressures and impacts on aquatic systems, and implementation of remediation measures where waterbodies are considered to be at risk of failure to achieve their environmental objectives.

The technical requirements of the WFD that necessitate scientific support are outlined mainly in Article 5 (Characteristics of the River Basin District) and its associated Annex II, Article 8 (Monitoring of surface water status, groundwater status and protected areas) and its associated Annex V, Article 11 (Programme of Measures), Article 16 (Strategies against pollution of water) that addresses listed substances, and Article 17 (Strategies to prevent and control pollution of groundwater) and its associated, and forthcoming, Groundwater Daughter Directive. Detailed analysis of catchment characteristics, assessment of risk to surface and groundwaters, further analysis of existing information and collection of new data are all needed to support the implementation of the WFD. However, there is still much to understand about the relationships between the catchment and the movement of pollutants, and the response of the aquatic ecosystem to anthropogenic impacts. Internal catchment processes, dominant pathways of pollutant load and hydromorphology are all important for the response of aquatic biological communities to pressures that arise within the catchment. Understanding these relationships is further restricted by the inherent complexity of natural systems. The simplification of that complexity through the identification of key variables and responses is a valuable tool that can help realise the technical requirements of the WFD. Such *modelling* is a likely feature of implementation of all of the technical Articles that can support the overall objectives of the WFD (Article 1) to meet the environmental objectives outlined in Article 4.

A conceptual framework identifying the Drivers, Pressures, State, Impact and Response (DPSIR), within which to apply modelling techniques, can help clarify the relationships between components of ecological change in aquatic systems and the wetlands that depend on those systems. The links between the components of the DPSIR framework equate to an assessment of the risk of enhanced pollutant mobility, the effect of a hydromorphological alteration, and the response of biological elements. Adoption of a well-structured assessment of risk, coupled with appropriate models that can be applied to explore management scenarios is an important tool to assist with meeting the environmental objectives of the WFD.

The Main Report identifies and reviews many situations where mathematical modelling can be a useful tool to assist in the understanding of hydrological and chemical transport and processes that occur in catchments, and the ecological response to anthropogenic alterations that affect them. A key point in the application of mathematical models to support the implementation of the WFD is that they should be useful and relevant to management objectives, which themselves need to be well defined. The Main Report addresses general considerations important for the application of modelling in the implementation of the WFD and, through numerous examples, details of modelling approaches used in the catchment as a whole, and in each of the waterbody classes: rivers, lakes, transitional and groundwaters. Coastal waters are addressed only briefly. The Main Report is supplemented by an extensive annex that details individual models and sources of further information. It has been produced to enable hyperlinking between relevant sections and with an annex that provides further information on most of the models that are referred to. In some cases, this was not possible as detailed information was not found, or available. In any case, the comprehensive reference list in the Main Report allows sourcing of the relevant primary literature. There is also a range of large EU projects that consider in detail the application of modelling in support of the WFD. These are listed in Table 1.2 of the Main Report, and are hyperlinked to respective URL sites.

1.1 Objective of the Study

This project was based on the belief that effective implementation of the WFD requires well-focussed mathematical modelling, which needs to be simple in its application and/or well supported by appropriate expertise. The objectives of this study were to produce an assessment of the application of mathematical modelling for the implementation of the Water Framework Directive, and particularly those aspects of modelling that need to be prioritised within the prescribed implementation timetable (see Table 1.1 of Main Report). The objectives of the study were to:

- identify, and categorise by generic type, models of potential use for the WFD in Ireland and with due regard to the application of modelling for this purpose in other EU countries;
- provide a review, and recommendation for the use, of models to assess risk of catchment activities to quality standards in waters;
- review application of models for the identification and quantification of important internal processes that impact on the ecological quality of surface waters and the chemical and quantitative status of groundwaters;
- recommend best practice for use of large data sets in each waterbody type;
- examine the Artificial Intelligence (AI)-based models developed for use in England and Wales and assess the potential of these techniques for the development of models based on Irish data;
- identify and critically assess models of potential use in order to make recommendations for cost-effective use and development of models to assist with the implementation of the WFD in Ireland; and
- to assess the information requirement of the WFD, with particular reference to the proposed GIS Data Model as the perceived primary conveyor of information, to determine those information components which may be best provided by mathematical modelling.

2 Information Needs and Application of GIS

The implementation of the WFD includes the extensive use of Geographical Information Systems (GISs) that can assist with catchment characterisation and overall reporting requirements. The reporting obligations required under the WFD can be viewed as an information matrix, comprising a series of cells, each requiring information. The GIS data layers are highly appropriate for the storage, analysis and reporting of such information. The coupling of GIS and mathematical modelling is used increasingly to interrogate catchment-scale data sets. GIS is now well developed to assist catchment characterisation in Ireland (Section 2.2 of Main Report), with the potential for extensive use in the identification of hydrological pathways and, through linked physical and chemical data sets, of the potential impact on surface and groundwaters. As discussed in Section 2.2 of the Main Report, an important consideration in the application of pressure–state models is choosing the appropriate level of detail for the analysis. This should be guided by the requirements of the specific WFD task being undertaken. For example, the WFD Article 5 requirement for assessment of 'pressures and impacts' during River Basin characterisation may be most appropriately achieved by a 'screening level' assessment.

It is anticipated that the resolution of data sets within the 'Interfluve' Class should be appropriate to support different scales of investigation and data aggregation. Determination of the appropriate aggregation should be based both on the level of analysis required (e.g. screening or investigation) and on the characteristics of the data sets that describe a particular 'interfluve' zone. The established concept of hydrological response units (see Section 3.3.2 of Main Report, 'Hydrological Response Unit'), which aims to identify areas with similar physical and land-use characteristics which can be considered homogeneous for the purposes of modelling, provides a useful approach for practical data aggregation. Development of an approach for the creation of such hydrological response units, at scales and detail relevant to the implementation of the WFD, should be a priority for modelling and understanding the transfer of water and contaminants from the land to surface waters and to groundwaters.

Within relevant model domains, the output from modelling activities, whether spatially extensive (e.g. map layers), as time series (e.g. time series hydrographs and entrained loads or concentrations) or other, should be stored in databases whose formats can be accessed and displayed in the GIS together with the other GIS Data Model classes. Within the EU Common Implementation Strategy (CIS) Guidance document on GIS, optional database fields have been identified for certain key hydromorphological elements for surface waterbody categories. Hydromorphological elements, per waterbody category (see Table 2.2 of Main Report) can be expanded to incorporate required GIS elements (see Table 2.3 of Main Report).

GIS support for Pressure–State models can encompass a broad range of models of transfer of water, and associated particles or solutes, through catchments to receiving waterbodies. Of the four modelling domains, it is the most established and has the longest history of development. Given its broad spatial coverage (complete River Basin areas), it is particularly reliant on map-based information and, consequently, on GIS data sets. It is also particularly relevant to the interfluve area. Appropriate *surveillance*, *operational* and *investigative* monitoring is required by the WFD. GIS can assist in evaluation of the suitability of the current monitoring networks, in particular with regard to adequate coverage and representation of variability for surveillance purposes, and in the design of long-term operational and investigative monitoring through the visualisation of spatial patterns in pressures, risk and impact.

In support of the implementation of the WFD, GIS supported State-Impact models are relevant for assessment of ecological status. The data requirements of such models often include determination of loading functions or other physical factors which may be assisted by GIS data sets and GIS-based analyses. For example, the Physical Assessment Protocol of the AUSRIVAS modelling scheme utilises an extensive list of hydromorphological 'control variables' which are determined from GIS analysis. Other models may require information on different hydromorphological factors (e.g. residence times) or the factors used to determine waterbody type (Section 2.4.1 of Main Report) for modelling the response of the waterbodies to the inputs.

The application of Artificial Intelligence (AI) techniques to the interpretation of biological and environmental data is presented in Chapter 4. A fundamental premise of these models is that experts employ two complementary processes of plausible reasoning and pattern recognition, which can be simulated by the utilisation of AI-based methods. It is highly likely that a 'mental mapping' or 'spatial' context exists in the mind of an expert during evaluation of environmental systems and hence this spatial dimension is at least implicitly involved in any such assessment or decision-making process. This is the fundamental argument that underpins the use of GIS and leads to the conclusion that the 'spatial dimension' should form part of the reasoning and pattern recognition processes undertaken within AI systems.

3 An Overview of Models

3.1 The Hydrological Cycle and Hydromorphology

Implementation of the WFD requires an understanding of the entire hydrological cycle. Modelling within well-defined domains of the cycle have assisted greatly in the understanding of hydrological pathways. Within each of the domains identified where model use is either essential or potentially useful, there are often a number of models that could be applied. Model choice should take account of factors such as applicability, data demands and cost.

Hydromorphology and typology determine the rate of movement of material through waterbodies and the response of ecological systems to anthropogenic disturbance. Modelling of hydromorphology is implicit in hydrological models, since much of hydrological modelling is concerned with predicting the consequences of change in land or water use in the catchment and hydrological networks. Useful modelling of river and floodplain hydromorphology includes prediction and understanding of the effect of water pulses along a channel, and quantification and assessment of the effects of high (flood) and low (drought) flows. Models that simulate patterns of geomorphology or habitat succession and replacement are valuable tools for river and floodplain assessment and management. Simple models that relate biotic communities to characterisation of mesohabitat structure have good potential for cost-effective assessment of effects of physical changes in rivers, lakes and transitional waters. Indicators of Hydrological Alteration (IHA) to characterise inter- and intra-annual flow regimes can be used to define the magnitude of flow, the timing of occurrence of key water conditions, the frequency of occurrence of conditions, the duration of each water condition, and the rate of change of water conditions. The River Habitat Survey provides a useful methodology for assessment of hydromorphology.

Models based on hydraulic equations, and used with hydrological inflow series and channel cross-sectional data, can predict water levels, flow velocities and scouring. Models that predict water levels are often associated with engineering design projects, and relate to changes of a single dimension of depth (e.g. SWMM, HEC-RAS). Their usefulness in relation to the WFD relates to their ability to model and design/manage water flow conditions at specific locations or in specific reaches. For ungauged channels, models such as Micro Low Flows (MLF) can assist with estimation of flow alterations arising from, e.g., irrigation or water abstractions. Low flow models should be further investigated for applicability to the estimation of impact on ecological indicators and reference conditions, and to develop flow duration curves for ungauged sites. Where there have been hydrological distortions to the flow regime, a model developed for WFD application in Scotland, the Dundee Hydrological Regime Assessment Method (DHRAM) may be useful for application in Ireland.

Hydromorphological modelling techniques applicable to the WFD require further development. There is, however, clear potential for the extensive current and historical data of the Irish OPW to be 'mined' in order to develop a system similar to that of the IHA. Models that assess changes in the hydromorphology of lakes will predict the effects of changes in land use and water regime on flow, water level, residence time, connection to groundwaters, lake depth variation, substrate structure and shoreline features. Regression analysis between Q (water discharge rate) and ADA (lake catchment area) may prove useful for application to Irish lakes. Comparison of theoretical, from run-off precipitation estimates, and measured Q can provide useful insight into loss to groundwater, particularly in karst and semi-karst areas. The DHRAM incorporates a method to quantify the degree to which the flow regime of a river, or the level regime of a lake, expressed in terms of variables that are significant to ecology, departs from the natural condition, as well as a method for calculating anthropogenic alteration of water levels. Along with the REGCEL model, it provides a simple cost-effective way to analyse hydromorphological changes in lakes.

Simple regressions from topographical maps can be useful for estimating lake volume and, with estimated net precipitation, residence time. The tendency for a lake to stratify has important implications for residence times and simple models relating depth to length can indicate stratifying and non-stratifying lakes. Where hypsographic curves are available, these can greatly assist with determination of internal lake structure. Hypsographic curves for Irish lakes should be compiled and this information applied for estimation of residence time and lake physical structure. Simple modelling techniques to estimate mean depth and likelihood of stratification of Irish lakes need further exploration. Predictive models based on data readily derived from maps can also model quantity and structure of the substrate.

Shoreline habitat measurement is important for identifying possible causes of ecological impact because many lakes are impacted by development on or near the shore zone. Two US EPA schemes of particular potential for application to the WFD are: (1) Surface Waters Field Operations Manual for Lakes (FOML) and (2) the Habitat Measurement Programme (HMP). Further development and testing of mesohabitat assessment and models for lakes could provide a cost-effective aid to monitoring.

Hydromorphology of estuaries is affected by shape and saline intrusion. Most Irish estuaries are partially mixed. While there is some correspondence between the results of classification on topographical and salinity structures, the limits of estuarine type are inherently ill-defined. Estuaries are often classified according to residence or flushing time. This provides an indication of assimilative capacity, and is useful for comparisons among estuaries. Methods to compute flushing and residence times range from using gross estuary characteristics to detailed hydrodynamic and solute transport models. The effect of climate change will enlarge the vertical and horizontal extent of estuaries, resulting in the penetration of tides further upstream and resulting in alterations of sediment deposition. Many naturally occurring morphological changes and likely impacts from climate change are slow and may be insignificant during the first phase of implementation of the WFD. Anthropogenic impacts can, however, be significant, sometimes dramatic, over short periods of time. To quantify such changes it is usually necessary to carry out detailed computer modelling of some or all of: tidal dynamics, wave dynamics, wind dynamics, sediment transport and sediment budgets.

Pre-screening of English rivers for morphological changes, in relation to assessment of Heavily Modified Water Bodies has included use of the RHS (River Habitat Survey) and FDMS (Flood Defence Management System) data in conjunction with published maps, whilst screening for river reaches and lakes with altered hydrological regimes in Scotland was approached using the DHRAM. In Finland, assessment of the impacts of hydrological change on biology have included the REGCEL water level analysis tool.

3.2 Pressure–State Models and Model Structure

Pathways that describe *Pressure–State* may involve a number of steps and model domains. Models that attempt to estimate *State* range from the very simple, requiring crude estimates of catchment attributes or human densities to highly complex models. In general, landscapes are heterogeneous 'patchworks' in which spatial pattern and processes interact to produce domains in which either retention or transport of matter dominates. Catchment models are distinguished by (a) the precision of the spatial units used in analysis as being lumped or distributed and (b) the precision of the events modelled over time as being a single or continuous event. Application of catchment models should consider effects of temporal and spatial scales.

Issues of complexity are important in the application of models that range from highly detailed process-type models, which account for spatial and temporal patterns, to simple 'empirical black-box' models that, through a series of equations that describe net movement of nutrients or other substances of interest, are calibrated without detailed knowledge of transport kinetics. All models, however, require initial conceptualisation in order to provide a logical sequence of connections between model compartments. It is also apparent that the distinction between 'complex' and 'simple' can be a misnomer as the development of 'black-box' models evolves towards greater complexity and that of 'process' models to greater simplicity.

A distributed catchment model accounts for the spatial distribution of the important catchment characteristics. A major attraction of fully distributed process modelling is that it develops an understanding of hydrological processes through incorporation of the important principles. Distributed models generally require information on topography, channel network, spatial distribution of soil types/properties and of land use/cover and management practices. Many distributed models are already linked to GIS. Distributed catchment models permit the detail that might be required to target *operational* and to effect *investigative* monitoring (under Article 8 of the WFD) and have been aided by the development of digital spatial data sets for topography (digital elevation models) and hydrologically relevant geographic data such as soil descriptors. The SHE (Système Hydrologique Européan) and related models are probably the most widely known example of a distributed model. As with any such example, the spatially gridded structure leads to a high demand for data input and parameterisation and, equally, provides for an ongoing process of development to improve incorporation of key hydrological processes and deal with higher spatial resolutions.

Process-based semi-distributed catchment models are simpler than fully distributed ones, and assume a similar response of many grid cells that can, therefore, be modelled in an integrated way. The HBV model is probably the most successful of the semi-distributed models. TOPMODEL is another example that has been developed and applied in many environments, although its application does not extend to catchments with important groundwater contributions

An alternative approach to detailed modelling, often requiring long-term and continuous measurement of substance and hydraulic transport, is to estimate loads of nutrients or other substances from catchment geology, topography and land use. Such empirical modelling has commonly employed the use of export coefficients. These offer an attractive management tool that does not involve either long-term and intensive chemical and hydraulic measurements or the understanding of soil kinetics. If common export coefficients can be applied across a range of catchments to estimate in-lake concentrations of, e.g., phosphorus or nitrogen with high reliability, the need for widespread sampling and chemical analysis in lake monitoring programmes could be radically reduced. Tests of these models have often found that while nutrient export across a range of waterbodies is ranked successfully, the predictive power of the models can be modest. Nevertheless, the development of simple empirical relationships between key features in the catchment and lake nutrient status merit further development. Use of export coefficients to rank risk of surface and groundwater degradation provides a powerful management tool and is of direct use in catchment characterisation and risk assessment required under Article 5 of the WFD.

Alternative 'black-box' models include the use of knowledge gained from greater detailed study of catchment processes, such as P-desorption, or more detailed division of the catchment into functional units. Recent work in the UK has developed an empirical modelling of diffuse P export (P-Indicators Tools) with a conceptual framework of three layers – storage, mobilisation and hydrological connectivity – for which the data input of each can be expanded and refined as knowledge and information become available. The model is a synthesis of three existing modelling approaches and is designed to support management options. The SPARROW model developed by the US Geological survey uses spatially referenced regressions of pollutant transport to estimate compliance with water quality targets. The method predicts water quality metrics as functions of river channel and catchment descriptors, including measurements and parameters that describe point and diffuse pollutant loads, and includes coefficients for transport efficiency.

Simple export coefficient methods, such as relating average P-loss from land-use categories identified in CORINE, can be efficient risk assessment screening tools that support characterisation of catchments under Article 5 of the WFD. Use of more complex empirical models such as P-Tools and SPARROW can provide further detail necessary for identifying critical source areas, with application in operational and investigative monitoring (Article 8 of the WFD) in catchments where waterbodies fail or are at risk of failing to reach their environmental objectives. Other, conceptually simple, approaches for modelling land-use effects on water quality is the use of multiple regression models.

While general principles can be applied to the modelling of all material transported in water, there are also important distinctions between the transformations and transport mechanisms of some elements. Modelling of nitrogen transport merits consideration, quite separate from that of phosphorus. The common opinion that P is of prime importance for surface water enrichment of inland waters and that N is of greater importance in coastal and ocean areas is only true in a very general sense. The management and understanding of the mobility of both nutrients is important for the implementation of the WFD for the protection of surface and groundwaters from eutrophication. A conceptual model of the N cycle would generally be considered to involve a greater number of steps than that of the P cycle. While the movement of P through catchments and waters is basically a process of attenuation and onward, down-slope, mobility, that of N also links with the atmosphere. For this reason also, its management is of major consideration for climate protection as human activities have disrupted the global N cycle.

Point- and field-scale models of N movement (e.g. DRAINMOD-N, DRAINMOD/CREAMS) are primarily of research interest for understanding the processes and not applicable to the catchment scale. Large-scale catchment models (e.g. AGNPS, ANSWERS, N-LES, NLOAD, SOILN), estimating N loss to surface or groundwaters, have applied both a nutrient export coefficient and a more process-type approach. Models such as AGNPS consider separate land parcels as distinct, but hydrologically connected, and have been used widely in the US. A model can include a GIS Arc-Info interface, but is limited to single event simulation and to catchments not larger than 10 km^2. Recent work to link the nitrogen transport model SOILN and a soil and heat model SOIL into a modelling framework designed for management decision support is an example of an attempt to simplify complex models to facilitate more general use.

An N-leaching model, NCYCLE, is currently under development, with funding from Teagasc, for use in Irish grasslands. NCYCLE is an empirical mass balance model of annual N transformations in grazed and cut grasslands. It assumes that annual N inputs such as fertiliser additions, mineralisation and atmospheric deposition are balanced by the removal of N in animal product, losses to the environment through leaching, denitrification, and volatilisation and accumulation in organic matter. NCYCLE makes adjustments for sward age, climatic zone, soil texture and drainage status, with mineralisation rates increasing with age of sward, temperature, clay content and drainage. Limitation of these types of models may arise due to the inherent complexity of the processes involved in water movement and N cycling, and imprecision of data available as inputs. Like most mass–balance models it is insensitive to seasonal pattern.

Modelling of N runoff and impact has been progressed by the INCA model, which simulates flow, nitrate-nitrogen and ammonium-nitrogen and tracks both terrestrial and river flow pathways. The model is dynamic and can simulate daily variations in flow and nitrogen following a change in input conditions such as atmospheric deposition/sewage discharges or fertiliser addition. The model can also be used to investigate the effects of change in land use. Dilution, natural decay and biochemical transformation processes are included in the model as well as the interactions with plant biomass such as nitrogen uptake by vegetation. Development of a ‘sister’ phosphorus model INCA-P is in progress.

Further development of nitrogen-leaching models, especially in Irish grasslands, is required. Understanding of the processes is an important, although often difficult, challenge in order to implement sound management to meet the needs of the WFD and Nitrates Directive (91/676/EEC). The INCA model was developed specifically with the WFD in mind. Its application to Irish rivers should be investigated.

3.3 Water Flow Through Catchments

Movement of material thorough catchments is dependent on rates and pathways of water flow. In channels, the hydrodynamics of advection–dispersion and material transport underpin most simulation modelling. Open channel hydrodynamics can be represented in one, two or three dimensions. One-dimensional models are often used for analysis of a system over periods of years, and are frequently used to forecast overflow in sewerage systems. Two-dimensional models are employed usually where detail along the horizontal axis is required and where variation along the vertical axis has no significant influence, or is not required. If such is not the case a three-dimensional model is appropriate.

Water quality changes in rivers result from physical transport and biological, chemical and physical conversion processes. River models have traditionally considered changes in concentrations of substances along a river length to be consequential on advection + diffusion/dispersion + conversion processes. The best-developed models address point-source pollutants, and the current industrial standard is probably the CE-QUAL2E model. This model simulates dissolved oxygen and associated water quality variables and incorporates degradation of organic matter, growth and respiration of algae, nitrification, hydrolysis of organic nitrogen and phosphorus, re-aeration, sedimentation of algae, organic phosphorus and organic nitrogen, sediment uptake of oxygen, and sediment release of nitrogen and phosphorus. It assumes steady stream flow and steady effluent discharge and was not designed for temporal variations in stream flow or for where major discharges fluctuate over diurnal or shorter time periods. Other well-used models such as the Danish-developed MIKE11 are better able to simulate transient conditions.

Many of the principles and water-quality models used in rivers are also applied, or adapted for use, in estuaries. Water-quality models have been developed of many transitional and coastal Irish waterbodies over the past 20 years, using a variety of methods, but without inter-comparison to assess the suitability of particular models to Irish conditions; however, most general purpose water-quality models can be applied to Irish waters by specifying relevant boundary conditions and discharges.

The increasing emphasis on the importance of diffuse nutrient loads to surface waters and recent verification of the importance of field nutrient emissions from Irish catchments that lack any point sources highlight the importance of developing models that can simulate cumulative inputs and losses of nutrients in Irish rivers. However, given the difficulty in developing process models for that purpose, it is unlikely that such models applicable for widespread use in Ireland will be forthcoming in the near future. Furthermore, simpler nutrient models, such as SIMCAT used by the UK Environment Agency, that address point sources are generally applicable only if the contribution of point source dominates total nutrient loads. Recent and current upgrading of many SWT plants will reduce the contribution of many sewage treatment plants to total P load. Modelling may, of course, still have an important role in determining whether investment in P-removal technologies is required in order to meet compliance targets.

3.4 Modelling Nutrients in Lakes

Modelling nutrients and particulate transport in lakes has usually employed 'Vollenweider' type mass–balance models. While these models provide useful summaries of average concentrations, they do not, typically, account for seasonal variation in phosphorus flux, bioavailability of TP, internal loading of phosphorus, and patterns of phosphorus retention in lake water through seasonal mixing and stratification. Seasonal factors have major implications for the modelling of phosphorus in lakes and, more critically, the biotic response to those concentrations. The internal release of phosphorus from sediments further complicate the interpretation of mass–balance models, particularly in nutrient-enriched lakes prone to stratification. Application of Vollenweider steady-state models is best when applied to specific lakes, rather than as a generic regional model. A variety of alternative approaches have been suggested that address these difficulties. These include the use of sparse data sets, which are often a reality of monitoring and *post-priori* modelling. Use and development of such techniques will strengthen reliability of results.

Acid deposition in areas of low buffering capacity reduces the pH of soils and waters and can cause leaching of aluminium which impacts upon freshwater ecological communities. Reference conditions for acid status can be derived either from a calculation of Acid Neutralising Capacity using empirical relationships with non-marine cations and dissolved organic carbon or, in lakes, from diatom frustules preserved in sediment cores (see section on Palaeolimnology in Main Report). Models for assessing deposition of SOx and NOx include MAGIC, MAGIC-WAND, MERLIN and PROFILE. These have been used to address the impact of deposition and are long-term, process-based models used for assessing emission scenarios. Recent developments (MAGIC7) have linked soil nitrogen and carbon pools to acidification and enabled simulation of short-term episodic responses of mixing fractions of water coming from different pathways.

Computer models that analyse dangerous substances in aquatic systems are often very specific to the compound in question and habitat parameters. Application of models to Irish conditions requires verification that the chemical status and other habitat conditions (for example hydromorphology) are comparable with the modelled situation, and potential combined effects with other chemical substances present in the water have to be taken into account. Assessment of dangerous substances and modelling related to them in aquatic systems require further consideration for applicability and development in Ireland.

3.5 State–Impact Models

To understand the link between *State* and *Impact* of a pollutant, and to effect management, it is necessary to demonstrate reliable dose–response relationships. This drives the determination of Effect–Load–Sensitivity (ELS) models and the subsequent determination of *Critical Loads* and management of *Maximal Allowable Loads*. Such concepts drive water quality monitoring programmes required under the US Clean Water Act and are of fundamental importance for the implementation of *programmes of measures* under the WFD. Understanding of ELS relationships, relevant to all biotic elements, can be furthered through literature collations, awareness of ongoing current work and, where necessary, focussed new work. Lessons for use of models for determination and management of loads can be obtained from the US experience with setting *Total Maximum Daily Loads.*

State–Impact models are applicable for all biological elements listed in Annex V of the WFD, although development of models for prediction of ecological elements has been far less extensive than those relating to hydrology and nutrients alone. This reflects both a traditional emphasis on 'water quality', and also the inherent difficulties owing to spatial and temporal heterogeneity, food-web effects and the frequent lack of linear state–impact responses of biological elements.

The response of phytoplankton (usually measured as chlorophyll-*a*, but required under the WFD to include consideration of net cell volume of phytoplankton) to given concentrations of TP is variable, both between lakes and within years. Sub-annual time increments are especially important for predictions of phytoplankton production and standing biomass. New developments, such as the ecosystem model, *Lakeweb*, make this possible and the PROTECH family of models can simulate the growth and loss of phytoplankton in response to season, nutrient supply, grazing and wash-out losses.

Simple Vollenweider and multiple regression models to predict the response of algal populations in lakes to changes in nutrient loads could be applied without undue difficulty, given estimates of loads and hydromorphology. More complicated process models could be used for some lakes to guide programmes of measures where these are required. In particular, these models should be considered for higher profile lakes where a lack of understanding of the details of the processes and seasonal dynamics hinders management.

Humic substances leaching from land and decomposition of aquatic organisms, notably vegetation, impart colour to water. As colour affects the nutrient–algal response in many Irish lakes, this should be taken into consideration in modelling work. This will also help develop an understanding of the ecological mechanisms operating in coloured lakes. Current work in Ireland by N. Allott and E. Jennings (Centre for the Environment, Trinity College, Dublin) suggests that the GWLF model can be useful for predicting seasonal changes in colour, and nutrient inputs, of Irish lakes.

The WFD requires that macrophytes and other phytobenthos be used for the classification of surface waters. General models for predicting macrophyte distribution and community structure are not well developed, although there has been extensive work on studying the effects of pressures, particularly nutrients, on macrophyte communities. The use of general models for robust prediction of periphyton biomass is uncertain. Complex ecological interactions among components of the phytomacrobenthos (macrophytes, epiphytes and epibenthos), the phytoplankton, littoral invertebrates and zooplankton act against widely applicable use of mathematical models to help with WFD implementation. Site-specific models applicable to *investigative* monitoring and *programmes of measures* in Ireland require further research, although development of simple regression models linking periphyton with physical and chemical variables would be a relatively simple, and perhaps useful, endeavour.

The use of macroinvertebrates as indicators of river quality has a long history. This has included development of simple metric scores (as utilised by the Irish EPA for river quality assessment) that reflect individual species tolerance to pollution and, more recently, application of multivariate techniques, notably the UK RIVPACS, the Australian AUSRIVAS used to assess river quality, and the Canadian BEAST model developed to compare benthic communities in impacted and unimpacted sites in the Laurentian Great Lakes.

The USEPA has adopted widely the use of models for the classification of river water quality. These use a variety of metrics that cover an array of biological groups that, when integrated, provide an overall assessment of quality. The biometric approach includes criteria for reducing the number of metrics to the most relevant core group to be aggregated into a single quality score. Multimetric assessment can, however, provide a low predictability of correctly assessing impairment of a site and use of both multimetric and multivariate approaches provides for a better methodology. Multimetric and multivariate classification tools require comparison and further evaluation of their application to the WFD.

3.6 Fish

Linking fish habitat preferences to river hydraulics has been done in a number of models (e.g. PHABSIM, RHABSIM, RHYHABSIM and EVHA). While such models can be useful in determining the response of fish to discharge and features of the habitat, and can incorporate hydraulic simulation models to predict availability of suitable habitat, they are often site specific and require precise topographical and discharge measurements. Recent work that predicts fish habitats from hydraulic geometry appears suitable for application across geographic scales. Recent developments in Ireland have involved GIS application to assess suitability of coastal rivers for salmonids. Models relating fish communities to impacts have a high potential for application in Ireland.

3.7 Ecosystem Models

Modelling approaches that link components of the ecosystem and which incorporate food-web effects are, currently, not used in routine assessment that relate *State* to *Impact*. Indeed, in general the application of ecological models to guide management is not widespread. They are, however, used increasingly as research tools in, mainly, lakes, coastal and transitional waters. Models that describe or predict the ecological response of single biotic 'compartments', such as phytoplankton or invertebrates, to driving variables, such as nutrients, have had some success because they are conceptually simple and are often site specific. However, models that incorporate effects and account for interactions across trophic groups and pollutants are likely to be required increasingly in freshwater and coastal management. Recent developments of ecosystem modelling include the *Lakeweb* model, ECOPATH and, increasingly, the use of Artificial Intelligence. Models that examine non-linear response and complex dynamics within aquatic ecosystems require further research and development. Application to the WFD of these models is likely to be valuable for investigative monitoring and *programmes of measures.*

Under Article 10, the WFD requires a combined approach for point and diffuse sources of pollution. This philosophy should incorporate both the effects and the interactions of the effects of mixtures of pollutants on the Environmental Objectives under Article 4 of the WFD. Integrated modelling of the combined pressures of eutrophication and contamination of organic toxins is an area of increasing interest. Further development of integrated models, such as the EUTOX group of models (CATS-5, AQUATOX, GBMBS, IFEM, HOC and QWASI, that predict effects on ecological status from mixed pollutants will be important for the application of *programmes of measures* (Article 11) in some situations.

3.8 Alien Species

Introduction of alien species has impacted on the ecological quality of Irish surface waters. Mathematical models applicable to introduced species are not developed in Ireland and for many established species are of questionable relevance. For more recent and aggressive introductions, there is a clear need to develop mathematical models that can help predict increased range, abundance and management options.

3.9 Palaeolimnology

The WFD requires the definition of reference biological communities in surface waters, and the extent of departure from reference state. Reconstruction of historical conditions using modelled relationship and transfer functions is a potentially powerful tool to assist with the determination of reference conditions and assessment of anthropogenically induced change.

4 Artificial Intelligence

Artificial Intelligence (AI) has high potential for the interpretation of biological and environmental data. The River Pollution Diagnostic System (RPDS), based on pattern recognition, and the River Pollution Bayesian Belief Network (RPBBN), based on plausible reasoning, are recently developed models that can provide important support to the implementation of the WFD, with respect to identifying ecological status (see Annex V of the WFD). The RPDS is the more advanced of the two models and has a comprehensive user-friendly interface that gives access to many useful diagnostic functions. The RPDS identifies characteristic patterns of biological, physical and chemical stress. In addition to these two operational models, a theoretic pattern recognition system, MIR-max (Mutual Information and Regression maximisation), used for the development of the RPDS, is a user-friendly system for the development of diagnostic or prognostic models from data.

Under conditions of uncertainty, methods of ‘inexact’ or plausible reasoning, such as Bayesian inference, provide a powerful tool that enable: (a) the ability to reason bi-directionally (i.e. from cause to effect and from effect to cause as required); (b) the ability to modify the dependencies between variables whenever new evidence is introduced; and (c) the ability to change one’s mind when new evidence ‘explains away’ earlier evidence. The RPBBN is an operational River Pollution Bayesian Belief Network developed from the 1995 survey of rivers in England and Wales, and consists of spring and autumn samples for 3615 sites having biological, environmental and chemical data. The AI-based systems have been shown to be valuable diagnostic and prognostic tools that provide a sound foundation for the development of a robust WFD classification system as required under Article 8 of the WFD.

5 Groundwaters

The integrated catchment approach of the implementation of the WFD requires viewing groundwater as an element of a continuous system, with inputs from precipitation and surface waters, with linkages to surface waters and to ecological systems supported by these surface waters, and to terrestrial ecological systems dependent on groundwater. Chapter 5 of the Main Report reviews how modelling can be employed to help with many aspects of the requirements of the WFD as it relates to groundwater. In particular, it can assist with *Initial Characterisation* of groundwater bodies in each River Basin District under Article 5, and *Further Characterisation* of groundwater bodies identified as being at risk of failing to meet their Environmental objectives (under Article 4), which will establish a more precise assessment of risk in support of Programmes of Measures under Article 11. The type of characterisation required is inextricably linked with the evaluation of the pressure upon the waterbody, the resulting state of the waterbody and impacts upon it or linked ecosystems.

The purpose and scale of groundwater models are strongly interrelated. Processes may vary from simple one or two-dimensional flow in a waterbody to three-dimensional transport of pollutants. Groundwater models may be developed to solve problems at widely different spatial scales, from local scale (e.g. one- or two-dimensional simulation of flows within a 10 m radius of a well) up to regional- or catchment-scale three-dimensional simulations of flows. Modelling can be used to estimate the State of a number of groundwater receptors.

The Geological Survey of Ireland (GSI) has estimated groundwater vulnerability using a risk-based hazard-pathway-receptor framework. The hazard is provided by the pollutant activity and depends on the contaminant loading. The pathway and a qualitative probability of impact are combined in the groundwater vulnerability measure. Vulnerability is based mainly on the thickness and permeability of the subsoil and the rate of recharge. The receptor is provided by the aquifer (the groundwater resource) and by the presence of a major water supply well or spring (the source). While modelling pressure–impact has a limited role in *Initial Characterisation*, it has an extensive role in *Further Characterisation* and in the more precise estimation of risk to waterbodies.

All groundwater problems are three-dimensional, but three-dimensional modelling has large data and processing time requirements. The practical solution is to reduce the number of modelled dimensions from three to two, but this is only possible where the dominant characteristics of the hydrogeological system can be represented adequately by this approach. The choice of modelling software depends on availability of suitable model codes, ease of use, familiarity and cost of commercial products.

Pressure to Groundwater *State* models have been developed widely for predicting nutrient and pesticide concentrations in groundwater bodies, driven by needs such as the Nitrates Directive (91/676/EEC) and the Drinking Water Directive (74/440/EEC). The focus has been on nitrates, phosphorus and on groups of herbicides and/or pesticides. Nutrient (and pesticide) transport models for defining impact on groundwater can be classified into two broad categories: (1) loading models, which effectively define the source loading at the base of the root zone and do not treat any of the physical processes in the rest of the unsaturated zone or in the groundwater itself; and (2) process models that model the hydrochemical processes involved, both in the loading (root) zone as well as in the unsaturated soil–water zone and in the groundwater, saturated zone.

6 Models as Decision Support Tools

The use of models to support the WFD requires not only identification of appropriate models but also technical, and end-user, decision support mechanisms. This involves the integration of science within policy and enhanced methods of communication and understanding among scientists, decision-makers and stakeholders. The use of modelling for decision support includes forecasting the outcome of various scenarios and developing integrated frameworks for management. Such frameworks integrate the most appropriate existing models, data and knowledge and are employed commonly at regional scales. This is in keeping with the River Basin District approach of the WFD. Decision scenarios allow the exploration of the *probability* of impacts from alterations of current management and assist with policy development.

Quantification of natural states and processes include uncertainty, which can be accentuated in models that link processes together and incorporate insufficiently validated assumptions. The robustness of application of models to catchment management requires, at least, an awareness of model uncertainty, but this should not prevent the use of models. It is important that policy-makers and end-users appreciate the uncertain nature of the natural world. Otherwise, there can be unrealistic demands for certainty of model outputs and distraction among stakeholders about definitions of the problem to be solved.

Simple management-orientated models using functional or empirical relations can appear more feasible, if less accurate, options than complex models. The simpler models, however, generally lack the mechanistic detail of the process models and may provide less insight to the required, and targeted, solutions of any particular problem. The choice to use simpler models over complex ones requires careful consideration, and there is no point in applying a simple model if it is inadequate for the task at hand. Many complex models that address water quality and quantity have undergone considerable development over the last 20 years to provide 'user-friendly' front ends. On the other hand, there is no guarantee that a complex model provides a better, or more reliable, outcome than a simple one in all circumstances.

6.1 Conclusions and Summary

Overall, current modelling techniques are likely to be of particular importance for the implementation of the WFD in respect of:

1. Identification of risk to ecological quality from catchment pressures. This should form part of the Characterisation process under Article 5 and use recent developments in GIS coverage;

2. Hydrological regimes and estimation of annual nutrient loads;

3. Assistance with elucidation, assessment and choice of *programmes of measures,* which necessitates a case-by-case approach; and

4. Definition of spatial and temporal resolution of monitoring systems for identification of hydromorphology, and chemical and ecological status.

Further developments of modelling are required to assist with: (1) determination of reference conditions, which is a fundamental requirement that can be assisted by a variety of multivariate analytical techniques, and subsequent determining of departure from *Reference State* for ecological classification; (2) use of Artificial Intelligence techniques for assisting with determination of ecological status; (3) identification of appropriate temporal and spatial scales to model impact of catchment processes on pollutant loads; (4) modelling frameworks for selection and integration of models; (5) development of decision and user support, to include enhanced communication for widespread understanding and use of models and dialogue among stakeholders; and (6) modelling of ecological systems response to S*tate* changes and management measures.

Two fundamental underlying requirements for the application of models to the implementation of the WFD are how models can help understand and identify risks to waterbodies and how they can help define and target monitoring. The implementation of the respective Articles (5 and 8) need to be closely linked with each other and with *programmes of measures* required under Article 11.

The report identifies many areas where modelling can be employed to assist with the implementation of the WFD. In summary, key issues are:

1. Models are, by nature, simplifications of reality;
2. Management objectives need to be defined clearly to guide model use;
3. There are no universal models, and selection of appropriate models for specific tasks is critical;
4. Models are likely to be extremely valuable in the assessment of risk of waterbodies failing to meet environmental objectives and in support of *investigative monitoring*;
5. Risk assessment should employ models to target monitoring and *programmes of measures*;
6. Simple models are, generally, more likely to be used and understood than complex ones, but great care is needed to avoid inappropriate model use. Complex models applied with the necessary expertise or user support can be far superior where there is a need to address spatial and temporal complexities;
7. There needs to be an appreciation of the strengths, weaknesses and uncertainties of individual models, where used;
8. All models, and the measurements used to calibrate and validate them, have errors which need to be quantified and reported;
9. Catchment and hydrological models are generally better developed, and with greater consensus of applicability to the WFD, than ecological models;
10. As identification, prevention and reduction of impact are the pillars of the WFD, there needs to be a greater emphasis on the development and application of ecological models to support the implementation of the WFD; and
11. The determination of *Reference Conditions* and EQRs across waterbody types provides a major challenge for which the development and application of models can be usefully targeted.

CHAPTER 1 INTRODUCTION

1.1. The Water Framework Directive and the aims of integrated management of water systems.

In December 2000 the European Parliament and Council passed into law EC Directive 2000/60/EC establishing a framework for Community action in the field of water policy, commonly known as the Water Framework Directive (WFD). The WFD places water within the context of the catchment through the implementation of River Basin Management Plans (RBMPs), developed for each designated River Basin District (RBD). The WFD will be the effective document under which national legislation will address quality issues within rivers, lakes, transitional waters (mainly estuaries), coastal waters and groundwaters. It also addresses those pressures within the catchment that lead to deterioration or provide risk to water and its ecology. The WFD has major implications for the sustainable management of both terrestrial and aquatic habitats and requires an approach that necessitates considerable development in the understanding of pressures and impacts on waters and the response of aquatic systems to *Programmes of Measures* designed to restore waters of less than *good* status. There is, therefore, more than an implicit requirement to develop tools to predict the response of surface and groundwaters, and the ecological communities that depend on them, to both increases and decreases in anthropogenic pressures.

A central theme of the Directive is the requirement to assess ecological quality of surface, including transitional, waters and quantitative and chemical status of groundwaters. This needs to be done with due regard to natural variability and with respect to criteria that defines waterbodies on the basis of the extent of anthropogenic impact. The WFD, therefore, requires not only good scientific practice to measure quality and quantitative status of waters but also the understanding of the effect of changing pressures, including seasonal, on that status. This, in turn, will necessitate the development of technical expertise to quantify the relationship between anthropogenic and natural processes that drive natural systems and the response of systems indicators (as detailed in Annex V of the WFD) to those pressures. Because, on one hand, natural systems are complex, variable and invariably non-linear in their response to physical and chemical drivers and, on the other, there is a clear need to implement the WFD with cost effectiveness, the need to apply mathematical models to assist policy appears indisputable. While the Directive makes limited specific reference to the use of mathematical modelling for assisting with, for example, the definition of type-specific reference conditions (as outlined in Annex II of the WFD), any detailed consideration of the Directive leads to the conclusion that modelling is highly relevant to many aspects of the Directive (Table 1.1). These include the design of effective monitoring networks, the identification of pressures, the risk that those pressures present for environmental objectives, the determination and validation of quality scores and the implementation of *Programmes of Measures* to meet the environmental objectives.

A premise of the WFD is that the quality of aquatic systems in Europe is under decline. While the pressures that have driven that decline are generally well known, the understanding of ecological thresholds and type-specific response of aquatic communities to hydromorphological, physical and chemical change is often not. This uncertainty can lead to conflict of opinion and political reticence to effect alternatives to current catchment and coastal management. Lag-times between a pressure and impact, natural heterogeneity, physical and chemical buffering mechanisms, varying sensitivities in the response of ecological communities to pressures, and other epistemological limits to knowledge may seriously impede the understanding required for management.

The implementation of the WFD requires a holistic approach to catchment management that is effected through a more classical reductionism in order to understand salient physical, chemical and ecological mechanisms operating within each domain of the catchment. Within these various domains mathematical models should be utilised to provide synthesis of complex natural processes and to identify the likely response within and among domains of natural and anthropogenic changes. It is difficult to envisage cost-effective and meaningful management without such aids

1.2. Objective of the Study

This project was based on the belief that effective implementation of the WFD requires well focussed mathematical modelling, which needs to be simple in its application and/or well supported by appropriate expertise. The objectives of this study were to produce an assessment of the application of mathematical modelling for the implementation of the Water Framework Directive, and particularly those aspects of modelling that need to be prioritised within the prescribed timetable of implementation (Table 1.1). The objectives of the study were to:

- identify, and categorise by generic type, models of potential use for the WFD and with due regard to the application of modelling for this purpose in other EU countries;
- provide a review, and recommendation for the use, of models to assess risk of catchment activities to quality standards in waters;
- review application of models for the identification and quantification of important internal processes that impact on ecological quality of surface waters and chemical and quantitative status of groundwaters;
- recommend best practice for use of large data sets in each waterbody type;
- examine the AI based models developed for use in England and Wales and assess the potential of these techniques for the development of models based on Irish data;
- identify and critically assess models of potential use in order to make recommendations of a cost-effective use and development of models to assist with the implementation of the WFD in Ireland; and
- assess the information requirement of the WFD, with particular reference to the proposed GIS Data Model as the perceived primary conveyor of information, to determine those information components which may be best provided by mathematical modelling.

1.3. Project structure

This report was commissioned to provide guidance for the application of mathematical models to the implementation of the WFD. In order to do that it was necessary to have, or gain, a familiarity with current use of models in catchment studies and management. It was also considered necessary to provide an overview of why models are applicable to the WFD and, within various sections of the report, to describe briefly the types of models applicable to a particular question. Examples are provided of models that are in common usage and those that have, or may have, high potential to assist with WFD implementation. The number of models currently in use is very large so rather than incorporate description of numerous models within the text of the main report, in general, descriptions of many current models is given as a stand alone compendium produced as **Annex I** to the report. Where appropriate, there is a hyperlink in the electronic version of the report to model description. While the report does not provide a comprehensive review of mathematical models applicable to catchment management, which would likely require a large volume of texts, it does, as considered necessary, provide brief reviews of processes that drive transport of material or impact on ecological status of surface waters or quantitative and chemical status of groundwaters, and the models relevant to the description or prediction of those processes. Similarly, although the project did not attempt to develop new models, it has attempted to indicate where future needs may lie in model development that will assist the implementation of the WFD. The project has focussed on the application of models relevant to the understanding and prediction of anthropogenic impact from land-use. It does not address models associated with climate change or flood control. There are numerous studies and texts on climate modelling, which were considered outside the scope of the project. The UK Centre for Ecology and Hydrology has produced five volumes that deal comprehensively with flood prediction and management (CEH, 1999; http://www.ceh.ac.uk/).

Table 1.1. Important milestones in the implementation of the Water Framework Directive related, particularly, to where modelling may be needed.

Action	**Deadline**
Directive entered into force	2000
Identify River Basin Districts and competent authorities	2003
Characterise river basins	2004
Identify pressures and impacts	
Conduct economic analysis of water use	
Define reference conditions for good water status	
Identify locations and boundaries of water bodies	
Water monitoring programmes become operational	2006
Draft RBMP to be made public	2008
Programme of measures for achieving the environmental objectives to be identified	2009
Good water status to be achieved for all surface waters, artificial and heavily modified waters and ground water	2015
RBMPs to be reviewed and updated	every six years

There is an extensive and voluminous literature on mathematical models relevant to catchment management. Some recommended textbooks are: (Schulze and Zwolfer 1987; Thomann and Mueller 1987; Håkanson and Peters 1995; Singh 1995; Andersen 1997; Chapra 1997; Beven 2001; Westervelt 2001; Håkanson and Boulion 2002). Proceedings of a EurAqua meeting (Prieto 2001) reviewed the progress of modelling within a number of Member States in preparation for the WFD. One outcome of the meeting was an EU project, HarmonIT, which aims to develop a European Open Modelling Interface and Environment (OMI) that will simplify the linking of hydrology related models. This project is one of a number of EU funded initiatives

(EUROHARP, BMW, HARMONIQUA, HARMONIT, PAEQUANN, REBECCA) that are investigating a range of mathematical modelling approaches for WFD implementation (Table 1.2.). Similarly, a number of modelling tools have been recommended to assist with Section 303(d) of the 1972 U.S. Clean Water Act to meet objectives for drinking water, fishing and amenity value. The mechanism to achieve these targets is through designation of Total Maximum Daily Loads (TMDLS) and are discussed further in Chapter 3. See also (USEPA 1991; USEPA 1995; USEPA 1997; USEPA 1998; USEPA 1999).

Table 1.2. Current E.U. funded projects examining application of mathematical modelling to the implementation of the Water Framework Directive. The first four projects listed are within a larger cluster caller Catchmod (http://www.info.wau.nl/eesd1_1/)

Title of project	**Website**
BMW	http://www.vyh.fi/eng/research/euproj/bmw/homepage.htm
EUROHARP	http://www.euroharp.org/index.htm
HARMONIQUA	http://www.harmoniqua.wau.nl/
HARMONIT	http://www.harmonit.org/
PAEQANN	http://www.fundp.ac.be/sciences/biologie/urbo/paeqann.html
STAR	http://www.eu-star.at/frameset.htm
REBECCA	http://www.environment.fi/syke/rebecca

While this report draws on information available from the sources referred to above, plus extensive other literature and web-based material, its focus is on the mathematical modelling that can assist with implementation of the WFD in Ireland. It is, therefore, concerned primarily with characteristics of Irish catchments, or lessons from elsewhere that can be applied to Irish catchments. It is also cognisant of the scientific and political structures that will influence application of modelling within those catchments. Choice of potentially useful models are further guided by the Common Implementation Guidance Documents for the WFD produced at E.U level (Table 1.3.), and relevant experience of the use of models that support and guide policies in other countries, notably the US and Australia. The information needs for implementation of the WFD in Ireland are reviewed in Chapter 2. See also the website dedicated to the implementation of the WFD in Ireland (http://www.wfdireland.ie).

Table 1.3. Common Implementation Strategy guidance documents produced to assist Member States implement the Water Framework Directive.

Title
Identification of Water Bodies
Identification of River Basin Districts
Analysis of Pressures and Impacts
Development of a protocol for identification of reference conditions, and boundaries between high, good and moderate status in lakes and watercourses
Elements of Good Practice in Integrated Catchment management
Statistical aspects of the identification of groundwater pollution trends, and aggregation of monitoring results
Identification and designation of Heavily Modified and Artificial Water Bodies
Implementing the GIS elements
Economic Guidance
Public Participation

1.4. Why model?

The use of appropriate mathematical models can help describe or predict ecological processes and response to natural driving variables or anthropogenic pressures. Models can guide management and policies and help in the design of monitoring programmes and interpretation of the results such programmes generate. Models can fill gaps in empirical data. The principles of why mathematical models are useful to the implementation of the WFD is succinctly outlined by (Hession and Strorm 2000). Models can:

- Help understand complex processes operating within the catchment;
- Fill gaps in monitoring data;
- Identify sources of pollution;
- Predict system response to change; and
- Evaluate management alternatives.

The commonly adopted DPSIR (Drivers, Pressures, State, Impact, Response) framework can be applied to identify the modelling processes applicable to the WFD (Figure 1.1). The *Drivers* are activities in the catchment that lead to pressures on water resources. For many activities, as illustrated in Figure 1.1, these pressures are, typically, measurable pollutant loads. For example, a pressure from agriculture may be increased nutrient loads. Increased nutrient loads alter concentration in the receiving waters, the extent of which is dependent on *water body type*, determined by climate and character of the catchment. This defines water body hydromorphology. Hydromorphology can be altered through physical modifications of water courses (e.g. channelisation) or land (e.g. drainage). These factors collectively moderate the transfer of pollutant load to *in situ* concentration. This later factor can be considered to represent the *State*. It is for this reason that Characterisation of catchments, including the identification of water body types, is an important requirement (as described in Article 5) of the WFD. The link between Load and State often involves a series of mechanisms of varying complexity. The quantification of Load-State can be assisted greatly by mathematical models, and discussed in more detail in Section 3.3 of this report. Similarly, the effect of pollutant concentration on ecology is moderated by physical, chemical and biotic processes. These are often complicated and multifaceted and, again, mathematical models can be employed to quantify and predict *Impacts.* The translation of State to Impact also depends on hydromorphology, which requires monitoring under Article 8 and Annex V of the WFD (see section 3.2).

Some pressures may not, however, impact directly on chemical concentration, but directly on ecology. Pressures from abstraction of groundwater may impact upon quantitative supply of water to wetlands. Pressures from commercial fishing may have direct ecological effect on abundance and size structure of fish populations. Hence, while the DPSIR model provides useful guidance, it does not necessarily incorporate the whole Pressure to Impact sequence.

The *Response* within the DPSIR framework can be interpreted as synonymous with a *Programme of Measures*, as required under Article 11 of the WFD. A response to impact, can however, be implemented at each stage of the DPSIR sequence, as discussed below. Response can also be effected *in anticipation* of impact and based on risk analysis. The recognition of this option in catchment management is particularly important as a safeguard to high quality waters. A strategy of safeguard can, too, be assisted by mathematical models.

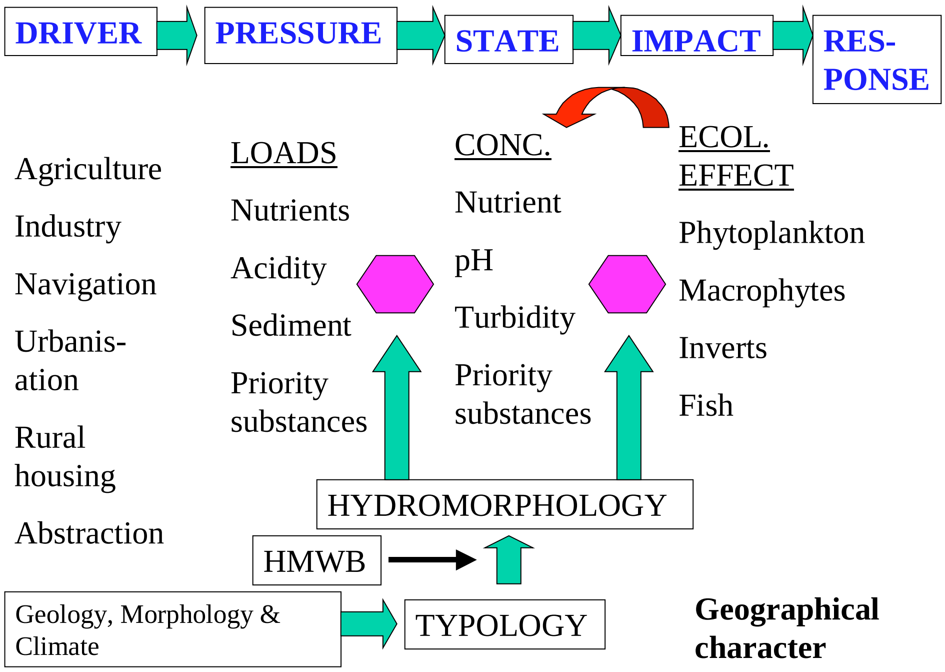


Figure 1.1. The Driver-Pressure-State-Impact-Response model of catchment management, with examples within the sequence. Shaded hexagons represent application of mathematical models. See text for further detail.

The application of the DPSIR framework can be either a clock-wise or anticlock-wise process. A clockwise process (Figure 1.2) is the more familiar, where one factor leads to the next, with the Response feeding back to the Drivers and the ultimate causative factors (often policies) or, as mitigating steps in other parts of the cycle. However, the framework can also be anticlockwise, with each step addressing the means of reducing the magnitude of the previous entity (Figure 1.3.). Linkages between entities can be scientific or societal processes and may be described by mathematical models, although the purpose and, therefore, details of such models are not necessarily the same for a clockwise (Figure 1.2.) or anticlockwise process (Figure 1.3.). Clockwise processes generally relate to and describe impact, and anticlockwise models, management.

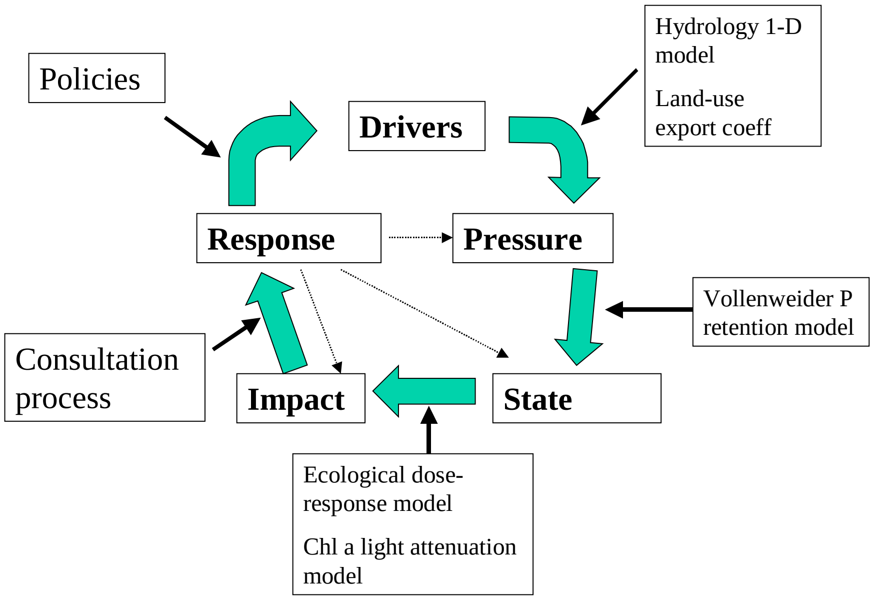


Figure 1.2.. An example of the input of mathematical models to the DPSIR framework of environmental management, in a clockwise direction.

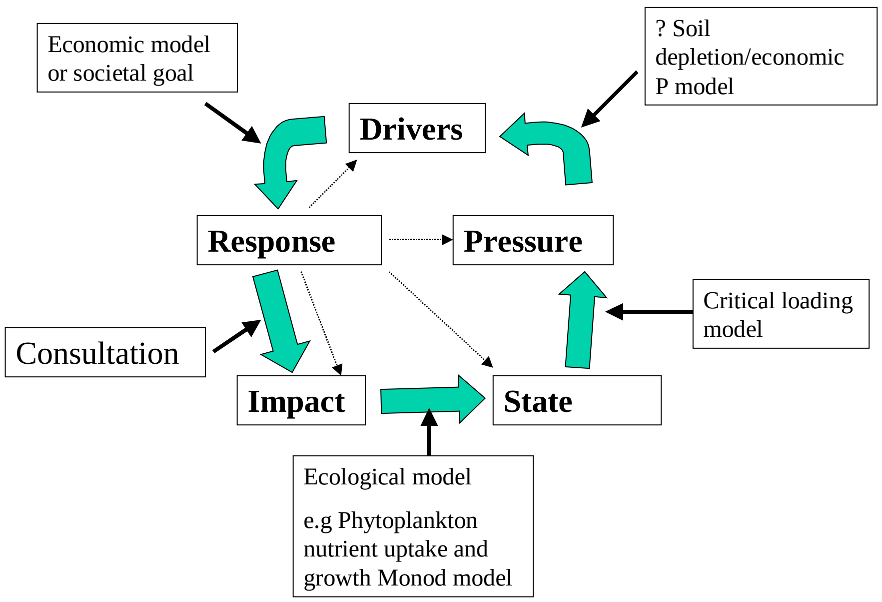
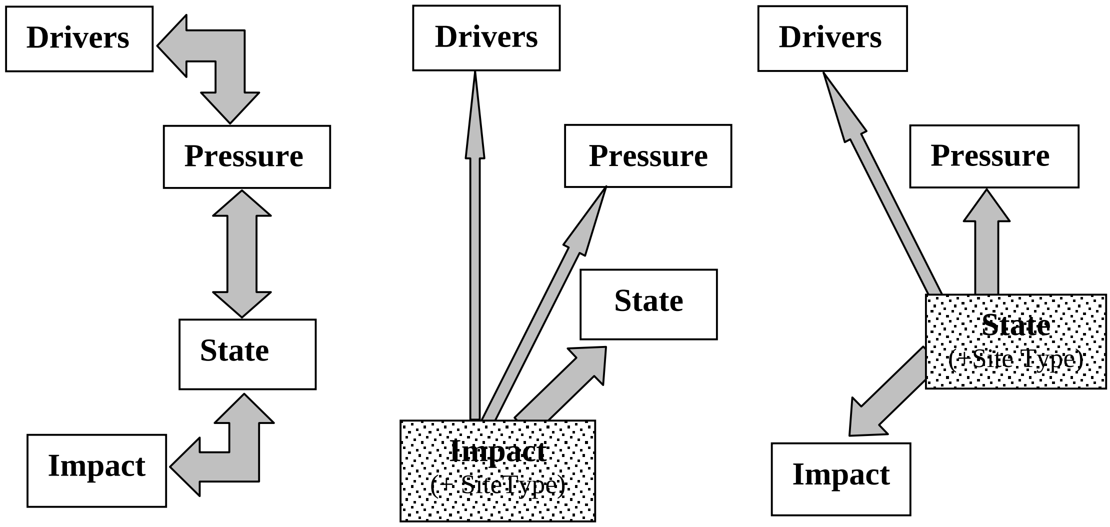


Figure 1.3. An example of the input of mathematical models to the DPSIR framework of environmental management, in an anticlockwise clockwise direction.

The application of models to particular aspects of catchment processes and management form the basis of Chapter 3 and Chapter 5. However, there are alternatives to a traditional process-orientated approach for the sequence of understanding relationships within catchments and our views of cause and effect reasoning.

Traditional process based mathematical models are well-suited to predictive modelling (i.e. from cause to effect - the clockwise direction shown in Figure 1.2.), but they are not well-suited to diagnostic modelling (i.e. from effect to cause – the anti-clockwise direction in shown in Figure 1.3.). Diagnosis invariably involves higher levels of uncertainty than prediction, simply because effect to cause relationships are more uncertain than cause to effect. However, the uncertainty about the likely cause of a particular effect (or symptom) provides valuable information, if expressed in terms of the probabilities of each possible cause. If other symptoms are observed the probabilistic evidence provided by each can often be combined to give a fairly conclusive diagnosis of the actual cause. Thus, the high levels of uncertainty in the model's internal relationships do not necessarily result in uncertain conclusions, provided the model handles them in a mathematically sound and consistent way. The first attempt to develop such a diagnostic model was in the field of medicine (Shortliffe, 1976). However, this was not based upon probability theory but on a modified rule-based approach, because the former had proved to be computationally too demanding. Fortunately, researchers in Artificial Intelligence (AI) made a major breakthrough (Lauritzen and Spiegelhalter, 1988) that facilitated the application of probability theory in mathematically sound and computationally efficient way, known as Bayesian Belief Networks (BBN). BBN represent the system domain as a network of causal relationships between variables and allow the user to 'reason' diagnostically or predictively. Thus, in the context of the DPSIR model, a BBN could be used in the clockwise and/or anti-clockwise direction to provide predictions and/or diagnoses, as illustrated in Figure 1.4a. Another AI approach to diagnosis, based on pattern recognition, has been developed and applied to ecological monitoring (Walley & O'Connor, 2001). In this case, patterns found in the combined biological and physical (or site type) data of a site are used to make inferences about its (chemical) state, pressures and drivers, as illustrated in Figure 1.4b. The reliability of the inferences (diagnoses in this case) deteriorates as the length of the cause-effect chain gets longer, as implied by the thickness of the arrows. This same type of model can be based upon exemplar patterns identified in other datasets. For example, Figure 1.4c shows how a model based upon patterns in the combined chemical and physical (or site type) data could be used to *predict* the impact on the biological community resulting from any given chemical/physical condition, and to *diagnose* its likely pressures and drivers. Since considerations for application of these types of models are a) fairly novel and b) could have major implications for the way management options to address impacts are formulated, we have included an extensive section of use of Artificial Intelligence models as Chapter 4 of this report.



(a) (b) (c)

Figure 1.4. Some possible applications of AI-based models, showing in (a) how predictions and diagnoses can be achieved using a single BBN model, and in (b) and (c) how they can be achieved using two different pattern recognition models, one based on patterns in the Impact (i.e. biology) and site type data, and the other based on patterns in the State (i.e. chemistry) and site type data.

1.5. Good and bad models

It is possible to predict an incorrect future with great accuracy or a correct future with great uncertainty (Beck 1987).

Models are, by their very nature, abstractions of reality used to simulate, rather than mimic, natural systems. They are seldom, if ever, truly correct (van Waveren, Groot et al. 1999) and application of models for management is often considered as much an art as it is a science. This does not imply a lack of rigour, but rather a recognition of inherent uncertainties and the need for the modeller to make intelligent choices in the development, use and reporting of models. This is both the strength and weakness of the modelling process. On one hand a model can reduce highly complex processes to simple output but, on the other, the strength of a model is determined by the relevance, and often extent, of the input data. Modelling can provide a powerful tool for management, but can be fairly meaningless if there is an ill defined objective, poor conceptualisation of the causative relationships and their uncertainty, or if insufficient attention is paid to essential technical aspects of the modelling process. Failure to address, or at least be acutely aware of, these issues restricts sensible interpretation of results.

Mathematical models fall into a number of generic types that assemble and use data in different ways. All models have a *domain*, which provides the boundaries within which they were designed. Operating outside the defined domain is ill-advised. Model development, however, often comprises hierarchical building blocks employing an array of methods and scales (e.g. bench scale, small field, laboratory mesocosm, field studies) in order to provide a conceptual model of the system (Kemp *et al*., 1995). A good conceptual model is essential for the successful application of modelling which, itself, can help develop the concepts. A major distinction often made between models is the division into the, so called, empirical models or the process models. Empirical models provide relationships between variables without taking into account the dynamics of the processes modelled. They are based only on statistical or judgemental summary of data (Reckhow and Chapra 1998) and generally predict the magnitude of a response variable to a change in a driving variable. Time-variant processes are not identified separately, but may be incorporated through amalgamation into long time-steps, such as annual means, to provide estimates of steady-state. In contrast, process (also known as dynamic or deterministic) models are very much concerned with changes of variables over time, commonly denoted as e.g. *dN/dt*, and generally depend on mathematical descriptions of the processes involved. They are based strictly on scientific theory with processes described typically by scientifically reasonable equations. For example, they may include in the model such processes as change in partitioning of a chemical between states (e.g. dissolved or adsorbed onto a particle) in response to ambient conditions or rate of transport through a system by, e.g. advection-dispersion. Spatial resolution of models is also important, with broad distinction between *lumped* and *distributed* models which describes the extent to which models addresses areas, such as land-use categories, as homogenous units as opposed to treating, and modelling, spatial units separately. Broadly, model complexity and data requirements, increase with spatial and temporal resolution. Existing models often link a number of domains and may include a mix of modelling approaches. (Ahlgren, Frisk et al. 1988) reviewed pros and cons of empirical and dynamic models for lake eutrophication studies. Dynamic models can provide better causal relationships, which can clearly guide management, but often it may not be possible to collect the extensive data needed to develop or apply them (Håkanson & Peters, 1995).

Everything should be as simple as possible, but not simpler (Albert Einstein)

The factors that guide the selection of an appropriate model or models relate to 1) applicability, 2) data requirements and 3) ease and cost of use, including necessary provisions for training. Complex mathematical models may not be transparent in their working and, therefore, difficult to explain to a non-technical audience. Models which require extensive and detailed data may not be feasible for operational purposes, unless they can reliably depend on one-off calibrations and validations. Simple models, on the other hand, may not be sufficiently intricate to be generally useful. For both complex and simple models, appropriate formulation of processes are important (Håkanson 1999), in order to provide a realistic conceptual model.

Applicability of models need to be guided by a realistic appreciation of what is required. Complex, data-hungry, models are not necessarily the best. Simple methods often suffice and are certainly appropriate where only rough or relative estimates are required and where overall estimates of annual net impact provides enough information to effect management (USEPA, 1999). Examples of simple methods would be nutrient export coefficient or simple regression models to predict nutrient loads (see section 3.3.3). These can help particularly with catchment characterisation under Article 5 of the WFD as part of the risk assessment process that water bodies may fail to meet environmental objectives as outlined in Article 4 of the WFD. Both aspects can guide monitoring programmes required under Article 8 of the WFD. Where a more detailed understanding is required, such as where a pressure may have important seasonal components but where there is, nevertheless, no capacity to apply very detailed modelling, the use of 'midrange' models (e.g. GWLF, AGNPS) might be employed (USEPA, 1999). In implementation of the WFD it could be envisaged that such an approach may be needed in some operational or investigative monitoring. The most detailed models need only be applied to help management if it is clear that explicit analysis and understanding of underlying mechanisms are required. This could include a need to know high resolution temporal or spatial patterns of behaviour or impact of a pollutant. Under such circumstances, explicit process models (e.g. QUAL2E, HSPF, MODFLOW 3) can be powerful tools (USEPA, 1999). Mid-range and complex modelling are likely to be required mainly for investigative monitoring (Article 8) and for the implementation of Programmes of Measures (Article 11) where the cause of the failure to meet the Environmental Objectives are uncertain or contentious.

A handbook on Good Modelling Practice has been produced by a Dutch consortium (STOWA/RIZA, 1999; accessible free of charge from: http://www.info.wageningen-ur.nl/research%20projects/gmp.htm). The Handbook focuses on numerical and process orientated models, but contains principles of general applicability to all modelling. It provides a seven-step format and checklist for wise use of models. In addition to describing, in broad terms, the components required for each step, it also highlights essential considerations for the use of models and some common pitfalls. General guidance relevant to application of models to support the implementation of the Water Framework Directive include:

- Define the objective that specifies the domain of the problem and the scenarios to be addressed;
- Determine if a mathematical model is needed to reach the objective;
- What reliability of model solution is required and does the expertise exist to apply the model;
- If a model is thought to be needed, provide a conceptual framework;
- Determine scope and boundary conditions, which guide data needs;
- Select a type of model;
- Verify that the conceptual model is effectively addressed by the computer programme chosen;
- Check the suitability or robustness of the model to extreme values of input data;
- Check the sensitivity of the model to changes in input values;
- Calibrate the model against empirical data sets;
- Validate the calibrated model with independent data; and
- Check if objective has been achieved (did the model answer the question that is was supposed to).

Failure to take account of any of these factors can result in a poor model output with limited descriptive or predictive value. For application to support the WFD, it may be tempting to use models which require data that, for whatever reasons, are not feasible to obtain or, conversely to use very simple models for which a very low degree of confidence can be placed in the results. Such models are not necessarily useless providing there is a realistic understanding of their strengths and weaknesses. But, inappropriate model use, or inexpert interpretation, can lead to results that lack credibility.

1.6. Model Uncertainty

A level of uncertainty applies to all models and application of any model should include testing and sensitivity analysis. Sensitivity analysis shows how variation of a single factor affects model outputs. Uncertainty affects data collection and all stages of the modelling process and tends to increase with both the number of processes that feed onto the model along the DPSIR chain, and with complexity within the relevant model domain. In predictive models, uncertainty arises from inherent variability in natural processes, model uncertainty and parameter uncertainty (e.g. (Vicens, Rodriques-Iturbe et al. 1975; Suter, Barnthouse et al. 1987). While the importance of uncertainty analysis is well recognised (e.g. (Reckhow 1994; Håkanson 1999) it is usually not included in pollutant transport models. This is a serious omission because if variability of input variables are large, so too will be output predictability. Beck (1987), (Håkanson 1999) and (Håkanson and Peters 1995) provide excellent discussion of this issue. If *within* ecosystem variability is large, many samples need to be analysed to provide a given, defined, level of certainty in a mean value. Combined spatial, temporal and analytical uncertainty may be particularly high for measurements of some of the most important chemical ecosystem drivers, e.g. total phosphorus. This has profound implications for the reliability of use of simple models that predict ecosystem response from, e.g. nutrient loadings. As Håkanson (1999) states "data from specific sites and sampling occasions may represent the prevailing, typical conditions [in the lake] very poorly indeed". Model uncertainty is clearly of importance in the conceptualisation of the process for which predictions are required. For example, a one-dimensional hydrological model would be expected to have greater predictive power than an ecological food-web systems model for lakes. Investigations into, e.g. nutrient response models, suggest that prediction errors in both empirical and mechanistic models are unlikely to be under $\pm$30% and can be more than $\pm$ 100% (Beck 1987; Reckhow 1994). However it is possible that the impact on modelling of individual error terms may be overestimated compared with combined effect of pairs of related parameters (Reckhow & Chapra, 1998). However, it is also clear that error estimation is often neglected when it should not be. Increasingly, however, techniques such as Monte Carlo simulation are applied to predict frequency distribution of variables, especially in sparse data sets (Shanahan *et* *al*., 1998). Further discussion of uncertainty and techniques to address this are given in (Cox and Baybutt 1981; Inman and Helton 1988; Chapra 1997).

Adoption of Quality Assurance techniques reduces overall uncertainty and should be incorporated at all stages of the modelling process, from collection and analysis of samples (Dines and Murray-Bligh 2000) to uncertainty analysis of model outputs (Håkanson 2001) and, perhaps, even at the stage of management decisions (Hofmann and Mitchel 1998). Quality assurance with respect to the use of models of benefit to the implementation of the WFD is the subject of the E.U. funded research project HarmoniQua (Table 1.2.).

1.7. Errors and classification schemes

The WFD requires that member states adopt reporting protocols that classify water bodies as either *high, good, moderate, poor or bad.* Classification will be based on a state-changed approach that assesses the departure of individual water bodies from a reference (*high)* state, defined by an Ecological Quality Ratios (EQR). Under the classification scheme currently proposed by the REFCOND CIS group there is likelihood for frequent misclassifications arising from inappropriate scoring of individual quality elements (Moss *et al*, 2003) and statistical probability functions**.** The errors associated with classification schemes can be alarmingly high. Therefore, an understanding of the errors associated with misclassification is needed so as to design and implement cost-effective monitoring and assessment programmes. Annex V of the WFD allows that where there are no sites at reference condition, other options may use historical data, modelling or expert judgement to estimate reference conditions for some indicators. Modelling may assist not only with the identification of reference but also how to handle the monitoring data that determines an EQR.

It is perhaps ironic that while the WFD has forced a move away from a spatial-comparative system using fixed-boundary water quality criteria to classify sites, it nevertheless appears to readopt a similar, and less transparent, philosophy through an EQR approach. A probability approach to site classification recommended by

(Premazzi and Chiaudani 1992) provided a better, but not generally adopted, option in respect of the (OECD 1982) type water quality classification schemes. Such an approach would also be a more realistic one for site classification under the WFD. The reporting requirements of the WFD, nevertheless, promotes classification where sites will be "shoe-horned" to fit within administratively convenient boundaries. The view of typologies and recommendation for GIS support confirm this as the current reality. Real systems are variable, often stochastic, and certainly non-linear. The models that mimic them, and the statistics that provide confidence to model results increasingly incorporate such inconvenient factors. Application of models to the implementation of the WFD needs to embrace, rather than ignore, uncertainty and the challenges that poses for interpretation and reporting. It is worth bearing this is mind, irrespective of the constraints of reporting.

1.8. Linking model domains

There is no single integrated model that can be applied universally throughout a catchment in order to meet the demands of the WFD, even if applied to specific types of waterbodies. BASINS (http://www.epa.gov/waterscience/BASINS/) is probably the most advanced attempt at an integrated catchment model, that nevertheless incorporates a number of submodels to model catchment run off (HSPF and SWAT) and water quality (QUAL2E) models. Catchment loading models AGNPS and GWLF also incorporate a number of submodels that address separate components of nutrient transport through catchments. The SOBEK family of models (www.sobek.nl) provide linkable modules for river and estuarine modelling. Whether incorporated under "one roof" or not, a modular approach to catchment modelling will probably remain the more attainable reality; whereby individual models are developed to operate independently within the relevant domain but such that they are able to link with other models within a wider multi-model system. This approach enables communication of models, and modellers, within catchments and is an important consideration in the EU funded HARMONIT project. In the Netherlands, adoption of a modular approach has facilitated cooperation among institutes, and this is considered to be a key factor in progressing the use of modelling in the implementation of the WFD (Blind, van Waveren et al. 2000). A modular approach does not, however, need to detract from a holistic view of the catchment and the cumulative impact that inherent uncertainties may have for either application of individual models or, comprehensive, catchment management.

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CHAPTER 2 INFORMATION NEEDS AND APPLICATION OF GIS

2.1. Introduction

Chapter 1 provides a rationale for the use of mathematical models in the implementation of the WFD and *inter alia* proposes a conceptual framework wherein model application can be considered (DPSIR - Drivers, Pressures, State, Impact, Response in both forwards and backwards schemas); an overview of the purposes of modelling -'why model'; and introduces critical issues in model application including uncertainty, domain applicability and the concept of error including error in classification schemes.

Chapter 2 builds on this approach by the consideration of these activities within a second conceptual framework of the overall WFD information or knowledge management domain. The WFD and its specified reporting obligations can be viewed as an information matrix in which a series of information cells have been identified, each of which requires specific information. Given that most of the information has a geographical component or context (an absolute or relative position in River Basin 'space') GIS, comprising data layers with associated attributes or descriptors, is a highly appropriate method for the storage, analysis and reporting of such information.

This Chapter reviews the WFD Information Domain from a GIS perspective, and the applicability of a GIS Data Model proposed by the EU CIS Working Group on GIS, with the aim to determine information needs and identify information gaps which may be best addressed by mathematical modelling techniques. It includes an overview of an extension of the EU GIS Data Model to better fit with the needs of the WFD implementation in Ireland.

As a general statement it can be proposed that the coupling of GIS and mathematical modelling has become a widely established method for the efficient application and utilisation of environmental models. The range of topics incorporating linked GIS/models has become very broad and relevant to the WFD. A well established example is the USEPA 'Basins' GIS system which tightly couples a GIS with the SWAT, Qual2 and HSPF water quality models. The link between these specific models and a GIS is currently also under development in Ireland (chapter 3, section 3.3.6).

2.2. GIS specification for the WFD (EU Level)

The WFD requires that Member States report a considerable amount of information in the form of maps. The most suitable method for the transfer of information will be in the form of GIS data layers (as recommended in Annex I and II of the Directive). To this end a WFD Common Implementation Strategy Working Group on GIS (GIS-WG) was established to deal specifically with issues relating to the implementation of a common Geographical Information System. This Working Group has developed a Guidance Document *Implementing the GIS Elements of the WFD* which has been adopted by the Water Directors and which provides a comprehensive GIS Data Model for the GIS reporting aspect of the WFD.

The WFD does not set out detailed technical specifications for the GIS layers. As a consequence, an important initial task of the GIS-WG was to achieve a common understanding on a range of issues such as the contents of the various maps required, scales and positional accuracy of data and the reference system and projections to be used. In addition, recommendations are provided on the standards for data exchange and access, and on the content and structure of the metadata to accompany each data layer.

A key output of the Working Group on GIS has been the realisation of the integrated *Data Model* for the components of the envisaged WFD common Geographical Information System. This model lists the primary GIS layers and associated databases as 'Classes' in the WFD Information Domain. The model has been developed using Unified Modelling Language (UML) notation which has become a standard methodology and is applied increasingly to the modelling and design of GIS and Databases. The UML diagrammatic notation used provides a logical model of the dataset components required, as defined primarily by the Directive itself, together with a comprehensive data dictionary to describe the attributes of the tables that will be contained within the model.

The GIS Data Model Classes are outlined in Appendix III *Data Dictionary* of the CIS GIS Guidance document. In addition, Appendix III of the Guidance document provides a list of mandatory and optional database fields associated with each Data Model Class. The Classes in the CIS GIS data model are presented in Table 2.1, wherein an assessment of the potential for mathematical modelling to assist in 1) mapping of the class 2) completion of a mandatory field and 3) completion of an optional field is also presented. It is proposed that these Data Classes and their component database fields will comprise the GIS element of reporting from each Member State to the EU under the WFD.

For the completion of 'information cells' in this GIS Data Model (Classes and component database fields) it is likely that mathematical modelling may become the preferred, or in some instances the only feasible, method to derive the required information for some of the database fields. Discussion of the role of mathematical modelling to fulfill such aspects of the GIS Data Model is considered in section 2.4 subsequent to discussion of an extension of the Data Model for the WFD GIS in Ireland in section 2.3.

Table 2.1. EU CIS GIS Data Model Classes and role of Mathematical Modelling

Class	Feature type	Geo-delineation [1]	Mandatory Field [2]	Optional Field [3]
CoastalWaters	Polygon	yes	yes	yes
EcoRegion	Polygon			
GroundwaterBody	Polygon	yes		
GroundwaterMonitoring Station	Point	yes *		
LakeSegment	Polygon			
LakeWaterBody	Polygon	yes	yes	yes
ProtectedArea	Polygon	yes	yes	
RiverSegment	Line			
RiverWaterBody	Line	yes	yes	yes
RiverBasin	Polygon	yes		
RiverBasinDistrict	Polygon	yes		
SurfaceMonitoringStation	Point	yes *		
Transitional Waters	Polygon	yes	yes	yes
CompetentAuthority	Table			
FWEcologicalClassification	Table		yes	
GWStatus	Table		yes	
MonitorGWBodies	Table			
MonitorLWBodies	Table			
MonitorRWBodies	Table			
MonitorTWBodies	Table			
PhysicoChemical Classification	Table		yes	
SalineEcological Classification	Table		yes	
SWStatus	Table		yes	

[1] - mathematical modelling can assist spatial mapping of the class
[2] - mathematical modelling can be used to complete a mandatory data dictionary field
[3] - mathematical modelling can be used to complete an optional data dictionary field
* - mathematical modelling can assist in the optimal distribution of monitoring stations.

2.3. WFD GIS Specification for Ireland

The adoption of the EU GIS Data Model provides a standard approach for management of geographic information during implementation of the WFD. In the first instance, the purpose of the EU model is to underpin data reporting requirements between River Basin District projects in the Member States and the Commission. This common data model can also accommodate, to a degree, data arising from related investigations and analyses within River Basin District projects.

An assessment of this EU common GIS data model comprises a key task of the WFD GIS group within the EPA with support from other organisations. Most importantly, given its focus on the reporting aspect between the Member State and the EU, it has been realised that the EU data model does not consider adequately many of the activities in the implementation of the WFD, particularly the River Basin Characterisation (of Article 5) and, ultimately, the investigation of processes which may underlie the failure of waterbodies to reach their Environmental Objectives under Article 4. These are activities wherein the application of mathematical modelling is most likely to be required

To provide a comprehensive GIS Data Model, more suited to the full suite of management and investigative aspects within River Basin Management Planning in Ireland, the EPA is coordinating an effort to derive a more complete specification for an appropriate GIS Data Model. This is in part based on *Guidelines for the Establishment of River Basin Management Systems* (DEHLG/EPA, 2000). *Inter alia*, this includes dataset creation both at a central national level (involving different State organisations, including EPA, National Parks and Wildlife Service and the Geological Survey) and within individual River Basin District projects, and is a topic for consideration within the WFD National Working Group on Characterisation and Reporting. In some cases collaborative effort has been made to develop standard datasets, (e.g. EPA and the Central Fisheries Board work on development of a river network dataset).

This revised or extended Data Model reflects an analysis of likely requirements. As such it is conceptual but can serve as a routemap for dataset development; and in several instances the datasets have yet to be developed. The main elements of the extended Data Model encompass:

- Additional conceptual elements including a formal framework for datasets concerned with 'landscape' processes as distinct from water bodies (e.g. sources of pressure and transfer of pressures to waterbodies via environmental pathways);
- Insertion of additional data base fields to Classes in the EU Data Model; and
- Insertion of additional Data Classes most notably with reference to River Basin Characterisation and Risk Assessment

'Landscape' level representation within River Basins

Conceptually, the EU GIS Data Model does not provide a complete coverage of the land surface of 'River Basin space'. The space filling logic of the data model only extends to three levels:

Member State	(where space is filled by one or more River Basin Districts)
River Basin District	(where space is filled by one or more River Basins), and
River Basin	(wherein only the space filled by Water Bodies is specified)

Consequentially, the GIS Data Model for Ireland has been extended at the River-Basin level to include an 'Interfluve Class' which represents the landsurface between Surface Water categories and which is underlain by the types of Groundwater Bodies. This hierarchy of 'Space Filling' elements in River Basin 'space' is presented in Figure 2.1. The Interfluve Class, in conjunction with the WaterBody categories, thus allows for the complete tessallation of 'space' within each River Basin accommodating:

- Local zones within the Interfluve Class would represent different terrain or landscape units and would inherit properties from different datasets in the data model: Topographic - from e.g. datasets on elevation, slope, aspect, curvature;
- Environmental pathways - from e.g. datasets on soils, sub-soils; and
- Pressure sources - from datasets on landuse activities, emissions, or intrinsic properties such as lithologies leading to increased acidification.

Whereas such topographic, environmental pathway and pressure source properties (and the relationships between these elements) can be investigated in great detail within small areas, this is limited by pragmatic constraints including available time and personnel resources and the resolution of available data. As such, a challenge is to determine an appropriate scale and surface area of zones within the 'interfluve' areas for analysis. In the context of the WFD the concept of 'appropriate scale' is not fixed in any absolute terms. Rather, it should be determined by the requirements of WFD implementation, and with due regard to issues of scale (see section 3.3.2, '*Issues of scales in hydrological modelling'*). Activities undertaken in fulfilment to the requirements of Article 5 for the preparation of Characterisation reports may suffice with a coarse level of investigation as a 'screening level' assessment. Conversely, investigations under Article 8, Operational and Investigative monitoring, and Article 11, the establishment of Programmes of Measures may, within particular areas, require a detailed resolution of data and the identification of small areas for analysis.

Many models exist for the analysis of land to water processes (section 3.3.). Such models operate at different geographical resolution and aggregation of source data (wherein fully distributed paramater and lumped parameter models represent extremes in resolution). It is anticipated that the resolution of datasets within the 'Interfluve' Class should be appropriate to support different scales of investigation and data aggregation. Determination of the appropriate aggregation should be based both on the level of analysis required (e.g. screening or investigation) and on the characteristics of the datasets that describe a particular 'interfluve' zone. The established concept of hydrological response units (see chapter 3, section 3.3.2, *'Hydrological Response Unit'*), which aims to identify areas with similar physical and land use characteristics which can be considered homogeneous for the purposes of modelling, provides a useful approach for practical data aggregation. Development of an approach for the creation of such hydrological response units, at scales and detail relevant to the implementation of the WFD, should be a priority for modelling and understanding to the transfer of water and contaminants from the land to surface waters and to groundwaters.

The majority of the datasets included in the extension of the basic EU GIS Data Model in the Irish Data Model address the description of Interfluve Class units (e.g. sources of pressures and environmental pathways between such pressures and receiving waterbodies). Sources of pressure are disparate but in many instances their geographical extent is represented by data sets from National Organisations (e.g. forestry, agriculture and EPA IPC licensing section). A more complex challenge is to determine the constitution (specific pollutants or other effects) and magnitude of the pressures represented by these dataset topics, and the representation of such datasets in the GIS for analysis. The characteristics of the environmental pathways (the susceptability effect) which may transfer pollutants or other pressure effects from their sources to eventual receiving water bodies also needs to be determined. This may be assisted by the datasets identified in the Interfluve Class, although a suitable determination of the environmental pathways properties may require appropriate mathematical modelling.

Additional Data Classes in GIS Data Model

Other categories of data classes for addition to the GIS data Model include:

- Administrative boundaries (Local Authorities, District Electoral Divisions, Townlands) which serve as boundary definitions and also representative areas for the mapping of many statistics;
- Further 'expressions' of surface waters such as variants of the river network to portray linear mapping of parameters such as typology and 'Q values', or extensions to the geometric detail of the river network to encapture local drainage features of importance; and
- Remote Sensing data. This category would include standard aerial photography; high resolution digital aerial photography, satellite, airborne lidar and hyperspectral sensing (see Box 2.1).

Box 2.1. Remote Sensing - sources of data

- Standard aerial photography is acquired by the Ordnance Survey, on a recurrent basis, and is available as a standardised data product in orthorectified format. As it completely covers the area within River basins it can be used for general assessment and also for the extraction of a diverse range of features not recorded within other datasets, for example areas of particular habitat type (Ekebom and Erkkila, 2003) and riparian zones and also potentially linear features such as local drains.
- High resolution aerial photography is acquired by low level fixed wing or helicopter flights but as it has restricted coverage is usually obtained along specific linear paths such as river corridors or coastlines. Examples of existing datasets include coastline imagery acquired by the Department of Communications, Marine and Natural Resources and river corridor imagery acquired by the Central and Regional Fisheries Boards.
- Satellite imagery is available in an increasing range of ground resolutions, spectral composition and time frequencies and is an increasingly valuable source of information for environmental resource assessment and mapping. The EU standard ’CORINE landcover’ dataset is derived primarily from Landsat Thematic Mapper and a revised version of this dataset has been published by the EPA in 2003.
- Airborne lidar data is used, inter alia, for very detailed topographic mapping and has application in flood corridor analysis. Sections of drainage systems in the vicinity of Dublin have been surveyed by lidar survey.
- Hyperspectral data, derived by the collection of data in a multitude of specific narrow wavelength areas, can be used to detect specific environmental phenomena including vegetation patterns and chlorophyll levels in water. A research project undertaken for the EPA ("Remote Sensing of Lakes - Improved Chlorophyll and Data Processing" (O.Mongain et al., 1999) obtained estimates of chlorophyll in some 360 Irish lakes

It is anticipated that the extended GIS Data Model will provide a more complete framework for the application of GIS for the WFD, wherein information arising from different mapping and investigative activities can be stored and utilised in a structured manner in relation to the other Data Classes in the Data Model. Although the Data Model is not yet complete, the main elements identified to date are presented in Table 2.2.

2.4. Model Domains

Chapter 3 discusses a schema of models and their potential application within tasks relevant to the WFD. This discussion of models has been set out under 4 sections:

- Hydromorphology & Typology;
- Pressure - State Models;
- State Impact Models; and in Chapter 4
- Artificial Intelligence.

The remainder of Chapter 2 discusses the potential application of GIS and the GIS Data Model Classes in support of these modelling domains. As a general aim, it is proposed that the output from modelling activities, whether spatially extensive (e.g. map layers), as time series (e.g. time series hydrographs and entrained loads or concentrations) or other, should be stored in database formats which can be accessed and displayed in the GIS together with the other GIS Data Model classes.

2.4.1. Hydromorphology & Typology

Hydromorphology concerns the physical structure of waterbodies and factors affecting flow regimes, water residence times and sediment dynamics. The WFD requires consideration of hydromorphology in the definition of waterbody and, where impacted, to impair ecological status. Within the EU CIS Guidance document on GIS, optional database fields have been identified for certain key hydromorphological elements for the surface waterbody categories. Whereas these database elements are optional they represent an evaluation by the GIS Working Group of key hydromorphological elements. In addition, whereas the guidance document does not provide a formal definition of these items, it is argued that as many are not available from existing sources, they may be estimated from GIS based or other forms of modelling. For example, hydrodynamic modelling of transitional waters can be used to determine key hydromorphological factors for such waterbodies.

A summary of the listed hydromorphological elements, per waterbody category (Table 2.2) is expanded to incorporate required GIS elements in Table 2.3. The levels of elements to be incorporated are summarised in Figure 2.1. The elements of the waterbody categories which are defined as polygons (coastal, transitional and lakes) are largely defined by metrics determined within the water body entity. Some of the hydromorphological elements for rivers, however, reflect the more obviously cascading nature of river systems and address the entire upstream river network. Development of a fuller suite of variables to describe the hydromorphology of rivers and their associated catchments (including catchment shape and slope factors) has been undertaken within an EPA ERTDI funded research project (Hydromorphology of Rivers) utilising GIS based techniques.

The elements for the definition of waterbody category typologies are defined in the WFD (under System "A" or "B") and reflected in the GIS data model. Many of the elements can be determined by GIS-based direct measurement or analysis, and considerable work has been undertaken by the EPA in the application of GIS for this.

The draft typology for rivers, in particular, has developed largely by using GIS data model classes on terrain, geology, landcover and rainfall.

Table 2.2. Waterbody category hydromorphological elements within CIS Data Model

Waterbody category	Hydromorphological element
Coastal	Current velocity Wave exposure Mixing characteristics Turbidity Mean substrate composition Retention time
Lake	Depth Mean depth Lake shape Residence time Water level fluctuation
River	Distance from river source Flow energy Mean width Mean depth Mean slope River morphology Valley morphology Mean substrate composition
Transitional	Current velocity Wave exposure Residence time Mixing characteristics Turbidity Mean substrate composition Shape character

2.4.2. Pressure - State Models

The Pressure - State models (chapter 3, section 3.3) encompass a broad range of models of transfer of water and, associated particles or solutes, through catchments to receiving waterbodies. Of the four modelling domains it is the most established and has the longest history of development. Given its broad spatial coverage (complete River Basin areas), it is particularly reliant on map based information and, consequently, GIS datasets. It is also particularly relevant to the interfluve area.

Many of the categories in the GIS Data Model can provide suitable sources of information for pressure-state modelling:

- Elevation, slope, aspect, flow direction, flow accumulation and curvature are represented in the "terrain" category;
- Soils, subsoils and groundwater vulnerability are represented in the "substrate" category;
- Forestry, landcover and landuse are represented in the "landuse" category;
- Monitoring stations for the waterbody categories are represented in the "monitoring" category;
- Point discharges are represented in the "point source" category;
- Landfills, mines and quarries are represented in the "landuse" category; and
- Waterbodies, and the river nwtwork suitable for network analysis, are represented in the "waterbody" category

As discussed in section 2.2, an important consideration in the application of pressure-state models is determination of the appropriate level of detail for the analysis. This should be guided by the requirements of the specific WFD task being undertaken. For example, the WFD Article 5 requirement for assessment of 'pressures and impacts' during River Basin characterisation may be most appropriately achieved by a 'screening level' assessment.

The current distribution of monitoring stations, utilised by different organisations and for different purposes, is most unlikely to meet the long-term requirements for implementation of the WFD. A structured approach to monitoring is presented in the WFD wherein surveillance, operational and investigative types are identified, each with its own role and function. GIS can assist in evaluation of the suitability of the current monitoring networks, in particular with regard to adequate coverage and representation of variability for surveillance purposes, and in the design of long term operational and investigative monitoring through the visualisation of spatial patterns in pressures, risk and impact.

The development of appropriate 'screening level' techniques has been an important topic for consideration by the WFD National Working Group on Characterisation and Reporting. This group has proposed that the characterisation process can be undertaken to a considerable degree by the overlay of appropriate datasets in the GIS and the use of relatively simple scoring methods (Working Group on Characterisation and Reporting - draft report "Pressures and Impacts Assessment Methodology" 12/8/2003). The empirical models discussed in section 3.3.3 may also find useful application in this level of investigation. For a 'screening level' assessment, the level of detail contained in many of the datasets may exceed immediate requirements, and use of simpler summary data sets may be sufficient.

On the other hand, specific investigations where waterbodies fail or are likely to fail to meet the prescribed environmental objectives, may require a more detailed insight into the underlying processes to help determine the appropriate remedial measures. In this setting, distributed catchment models and their linkage with in-stream hydrological and water quality models may be required. The input data requirements of such models tend to be greater and may exceed the detail held in the basic GIS data model, imposing a requirement for specific dataset collection.

Practical experience, over time, will be required to determine the overall suitability of the GIS data model datasets to support different levels of investigation and the types of modelling discussed in chapter 3.

2.4.3. State - Impact Models

In support of the implementation of the WFD, State-Impact models are likely of primary application within the waterbodies for assessment of ecological status and, the related, Ecological Quality Ratio. Examples of such 'response' models include habitat (fish) models, the relationship between chlorophyll and nutrient levels in lakes or more general purpose multivariate models to assess ecological quality which are discussed in section 3.4.3. The data requirements of such models often include determination of loading functions or other physical factors which may be assisted by GIS datasets and GIS based analyses. For example, the Physical Assessment Protocol of the AUSRIVAS modelling scheme utilises an extensive list of hydromorphological 'control variables' which are determined from GIS analysis. Other models may require information on different hydromorphological factors (e.g. residence times) or the factors used to determine waterbody type (section 2.4.1) for modelling the response of the waterbodies to the inputs.

2.4.4. Artificial Intelligence

The application of Artificial Intelligence (AI) techniques in the interpretation of biological and environmental data is presented in chapter 4. A fundamental premise of these models is that experts employ two complementary mental processes in their evaluation of environmental systems, namely *plausible reasoning* and *pattern recognition*, which can be simulated by the utilisation of artificial intelligence based methods.

It is highly likely that a 'mental mapping' or 'spatial' context exists in the mind of an expert during evaluation of environmental systems and hence this spatial dimension is at least implicitly involved in any such assessment or decision making process. This is the fundamental argument which underpins the use of GIS and leads to the conclusion that the ’spatial dimension’ should form part of the reasoning and pattern recognition processes undertaken within AI systems.

The use of GIS in the development and application of AI methods for assessing environmental systems can be considered, *inter alia*, as:

sampling and selection of data:

development of sampling methods, or extraction of subsets from existing datasets, to ensure proportionate spatial coverage and representation. For example, selection of observations to adequately represent the diversity in stream magnitude, site specific catchment area and local gradient in river systems.

determination of site ’type’ parameter:

determination of key physical descriptors, e.g. many of the characteristics used in Annex II of the WFD for the typing of waterbodies, which may form the causal (or parent) variables in Bayesian Belief Network based expert systems. GIS may be important, in particular, in the application of zonal functions for the development of descriptors, e.g. statistics on catchment landuse or the mean slope in a specific catchment area. For example, many of the input variables for the AusRivAS Physical Assessment Protocol, which is fundamentally an assessment of hydromorphological factors, are GIS based measures of the physical character of the contributing catchment areas rather than the specific sampling site.

plausible reasoning:

The determination of prior and conditional probabilites are aspects of plausible reasoning and as stated in chapter 4 " *may be derived subjectively by elicitation from experts or more objectively by data analysis, if a suitable database is available"*. GIS can comprise an aspect of such objective data analysis and at the same time inform the expert perspective through the visualisation of different source datasets in their spatial context.

visualisation and verification of outcomes:

Relationships in data determined by AI methods, including clustering, predictive (i.e. from cause to effect) or diagnostic (i.e. effect to cause) will require both assessment or verification, and incorporation into the overall decision support framework. Visualisation of such model outcomes in a GIS in conjunction with other spatial datasets, including contained temporal trends, can comprise an important element of this process.

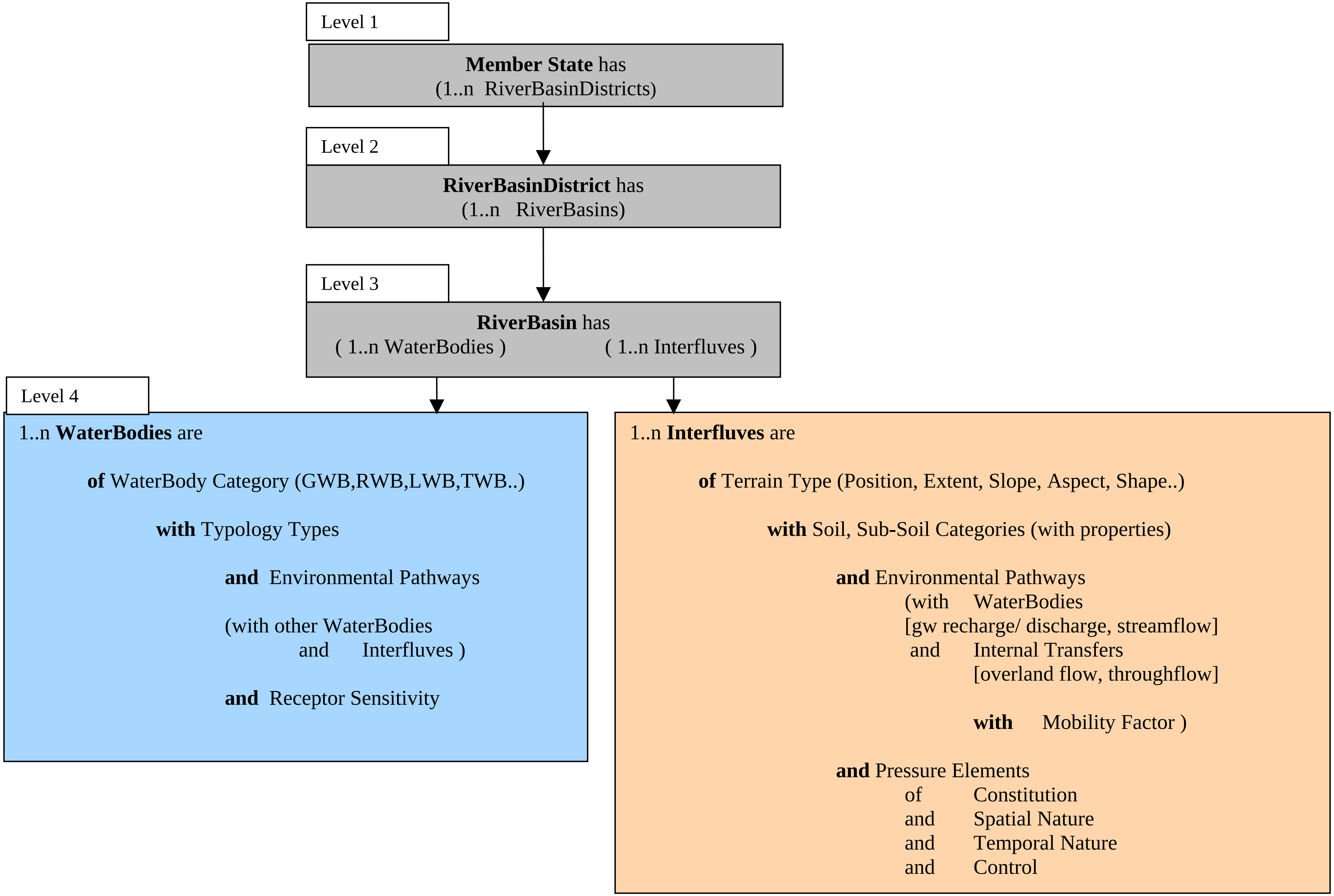


Figure 2.1 WFD GIS Data Model 'Space filling elements' Levels 1 2 3 and 4

Table 2.3. Main elements of the WFD GIS Data Model in Ireland

Category / Class	Class Name Prefix	Data Type	Source *
Boundary			
RiverBasinDistrict	RBD	polygon	EPA
HydrometricArea	HM_AREA	polygon	EPA
LocalAuthority / County	LAUTH	polygon	RBD /OSI
Sanitary Authority	SAN_AUTH	polygon	RBD /OSI
DistrictElectoralDivision	DED	polygon	RBD /OSI
Townland	TLAND	polygon	RBD /OSI
RegionalFisheriesBoard	RFB	polygon	RFB
RegionalFisheriesBoardDistrict	RFB_DISTRICT	polygon	RFB
CompetentAuthority	COMPAUTH	TABLE	DEHLG
EcoRegion	ECOREG	polygon	EU
RiverBasin	RIVBASIN	polygon	EPA
RiverSubBasin	RIVSUBBASIN	polygon	RBD
HighWaterMark	HWM	line	EPA
LowWaterMark	LWM	line	EPA
Water Body / Feature			
LakeSegment	LWSEG	polygon	EPA
LakeWaterBody	LWBODY	polygon	EPA/RBD
RiverSegment	RWSEG	line	EPA
RiverWaterBody	RWBODY	line	EPA/RBD
RiverMain	RWMAIN	line	EPA
RiverDrain	RWDRAIN	Line	RBD
RiverConfluence	RWSEG_CONF	point	EPA
RiverTypology	RWSEG_TYPOL	line	EPA
RiverQValues	RWSEG_QVAL	line	EPA
Hydromorphology	RIV_HYDROMORPH	TABLE	RBD
TransitionalWaterBody	TWBODY	polygon	EPA/MI/RBD
CoastalWaterBody	CWBODY	polygon	EPA/MI/RBD
GroundwaterBody	GWBODY	polygon	GSI
Aquifer	AQUIFER	polygon	GSI
ArtificialWaterBody	AWBODY_L	line	RBD
HeavilyModifiedWaterBody	HMWBODY_L	RBD	RBD
Monitoring / Classification			
SurfaceMonitoringStation	SWSTN	Point	RBD /EPA
GroundwaterMonitoring Station	GWSTN	Point	RBD /EPA
HydrometricGauge	HYDRO_GAUGE	point	RBD /EPA
HydrometricDischarge	HYDRO_Q	TABLE	RBD /EPA
MeteorologyObservation	MET_STN	point	RBD /ME
MonitorLWBodies	LWMON	TABLE	RBD
MonitorRWBodies	RWMON	TABLE	RBD
MonitorTWBodies	TWMON	TABLE	RBD
MonitorCWBodies	CWMON	TABLE	RBD

Table 2.3. continued

Category / Class	Class Name Prefix	Data Type	Source *
MonitorGWBodies	GWMON	TABLE	RBD
LaboratoryMonitoring	LABMON	TABLE(s)	RBD
PhysicoChemicalClassification	PCHEMCLS	TABLE	RBD
FWEcologicalClassification	FWECCLS	TABLE	RBD
SalineEcologicalClassification	SALECCLS	TABLE	RBD
SWStatus	SWSTATUS	TABLE	RBD
GWStatus	GWSTATUS	TABLE	RBD
Point Source			
UrbanWasteWaterTreatment	UWWTP	point	RBD
IPC_Licence	IPC	Point	EPA
Local Authority	LOCAL_AUTHORITY	Point	RBD
Stormwater	STORMWATER	Point	RBD
Farm_yard	FARM_YARD	point	RBD
Protected Areas			
Habitat	RPA_Habitat	Polygon	Duchas
DrinkingWater	RPA_Drinking	Point/ polygon	RBD
EconomicSpecies	RPA_EconomicSpecies	Polygon / line	RBD/MI/ RFB
Recreational	RPA_Recreational	Point/polygon	RBD
NutrientSensitivity	RPA_Nutrient	polygon	RBD
Substrate/ vulnerability			
Soils	SOILS	polygon	EPA/TEAGASC
SubSoils	SUBSOILS	polygon	EPA/TEAGASC
Bedrock	BEDROCK	polygon	GSI
KarstFeatures	KARST	polygon	GSI
RockOutcrop	OUTCROP	polygon	GSI
DepthToBedrock	BEDROCK_DEPTH	polygon	GSI
GWVulnerability	GW_VULNERABILITY	polygon	RBD
SurfaceRunoff	RUNOFF	polygon	RBD
Landuse			
Forestry	FORESTRY	Polygon	FS
Landcover	CORINE	polygon	EPA
MinesQuarries	EXTRACTIVE	polygon	RBD
LandFill	LANDFILL	polygon	RBD
LandSpread	LANDSPREAD	polygon	RBD
Land_Parcel	LPIS	Polygon	DAF
AgricultureCensus	AG_CSO	TABLE	CSO
PopulationCensus	POP_CSO	TABLE	CSO

Table 2.3. continued

Category / Class	Class Name Prefix	Data Type	Source *
Topography			
Contour	CONTOUR	line	RBD
Spot_height	SPOT_HT	point	RBD
DTM	DTM	grid	EPA
DTM_Fill	DTM_FILL	grid	EPA
DTM_FlowDir	DTM_FDIR	grid	EPA
DTM_FlowAccum	DTM_ACCUM	grid	EPA
DTM_Mask	DTM_MASK	polygon	EPA
DTM_Slope	DTM_SLOPE	grid	RBD
DTM_Aspect	DTM_ASPECT	grid	RBD
DTM_Wetness	DTM_TWINDEX	grid	RBD
DTM_Plan_Curve	DTM_PL_CURVE	grid	RBD
DTM_Profile_Curve	DTM_PR_CURVE	grid	RBD
HydroResponse	Hydro_Response	polygon	RBD

* source organisations
EPA -Environmental Protection Agency
GSI -Geological Survey of Ireland
OSI -Ordnance Survey Ireland
MI - Marine Institute
FS - Forest Service
CSO - Central Statistics Office
DAF - Department of Agriculture and Food
ME - Met Eireann
RBD - River Basin District Project (& constituent Local Authorities)
RFB - Regional Fisheries Board

CHAPTER 3 AN OVERVIEW OF MODELS

3.1. Introduction

Hydrologists use a conceptual model of the Hydrological Cycle (Figure 3.1.) to describe the nature and scope of the connection between the major stores, transformations and fluxes of water in the biosphere. These include Evaporation, Precipitation (rain, snow, hail), Evapotranspiration, Interception, Infiltration, Groundwater flow, and Surface runoff. The fluxes and transformations are driven by energy from the Sun. Implementation of the Water Framework Directive requires an understanding of the entire cycle and an operational capacity to address risk and impact of anthropogenic alterations to the transport of water and on life forms, including humans, that depend on that water. Depending on the purpose of the analysis only a part of the cycle may be studied but, even then, links to the others should not be neglected.

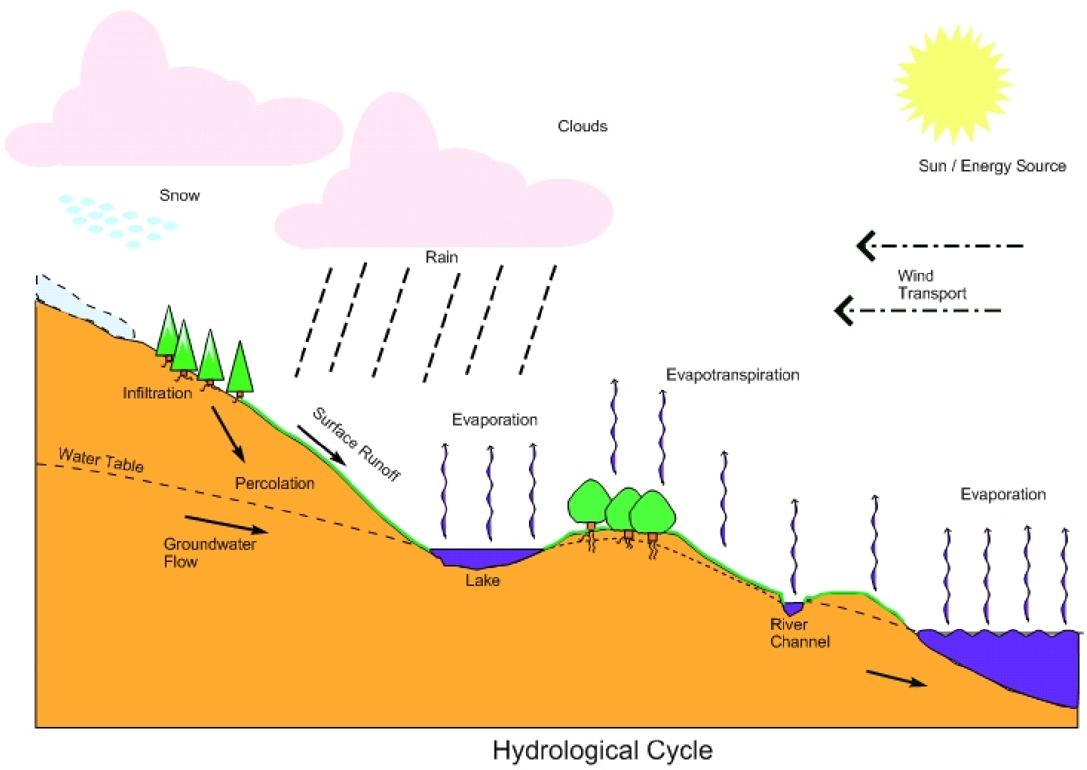


Figure 3.1. Representation of the Hydrological Cycle

Modelling relevant to the implementation of the Water Framework Directive can be applied to each stage of the hydrological cycle and to the linkages among those stages. Modelling is also applicable throughout the Drivers Pressures State Impact Response framework outlined in Chapter 1 (Figure 1.1). An early (2004) requirement of the WFD is a characterisation report for each River Basin District. This stage of the process relates Drivers to Pressures. Drivers provide a pressure through addition of a pollutant load or through a modification of hydromorphology, or both. In the DPSIR sequence, the first application of models are those that predict and/or progress understanding of the relationship between Pressure and State. While industrial impacts through point (e.g. outflows) or diffuse (e.g. acid deposition) are important for some localities or regions, the major pressure affecting Irish waters is land use that results in increased loads from land to water of nutrients, sediment, priority substances or acidity. Hydromporphology and Typology are important for the translation of Pressure to State and of State to Impact. The link between Pressure and State is driven by hydrology, and modified strongly by catchment characteristics and water body hydromorphology. These factors are also important, but to differing extents, in the link between State and Impact. Models that link Pressure and State are, in the main, driven by physical and chemical processes. Risk assessment of this link forms an essential part of the Characterisation Report, required under Article 5 of the WFD, and an area where modelling can be of particular value.

Pollutants are distributed through aquatic ecosystems by fundamental processes of inflow, diffusion, advection, sedimentation, burial, mineralisation, bioturbation and outflow. Modelling, therefore, applies common principles to their transport (Håkanson *et al*., 2003). All land-water transport models incorporate, though not necessarily in a transparent way, the hydrological pathways along which material travels: overland-, subsurface and differential- (including drain), and groundwater-flow. Computer based catchment models are, of necessity, gross simplifications of reality (see section 1.5). For example, modelling the movement through the catchment of the water in each drop of rainwater is neither possible nor practicable. Modellers therefore simplify in order to provide practical and useful tools.

Models that assist in the quantification of load emissions comprise two main families: the so-called process models, that account for the processes of substance transport, driven by hydrology and modified by the physical nature of the catchment, and the so-called empirical models that provide a summary of the relationship between categories of land-use and estimates of net loads. The distinction between these two families of models is not, however, always very clear with process models sometimes incorporating a "black-box" approach within the modelling framework, and empirical models that include variable hydrological parameters or sub-dividing landscapes based on their capacity to hold or transport material (e.g. mean slope, soil, geology).

The modelling of water movements and, to a lesser extent solutes and particles, have a comparatively long history (Singh, 1995). While biological processes in this link are easy to conceptualise, their incorporation into models is fairly recent and generally underdeveloped. The link between State and Impact is again affected by hydromorphology and physical and chemical transport of material but, more critically, by the biological response within receiving waters. As ecological response models are in general far less well developed than physical and chemical ones, there are many fewer "off the shelf models" than those that address hydrology and solute or particle transport. There is, however, increasing discussion about and development of ecological State-Impact models.

Within each of the domains identified where model use is either essential or potentially useful, there are often a number of models that could be applied. A comprehensive global model library is found at http://dino.wiz.uni-kassel.de/ecobas.html**.** Model choice should take into account factors of applicability, data demands and costs discussed in Chapter 1. As hydromorphology and typology of water bodies set the scene for so much chemical and biotic transformations, the use of modelling for these factors is addressed in section 3.2 of this report. This includes discussion of water level models. Section 3.3 is concerned with models applicable to Pressure-State relationships. Section 3.4 relates to State-Impact. Some modelling systems extend, of course, across those boundaries. Specific model descriptions are hyperlinked to Annex I and, where appropriate, from there to relevant URL sites.

3.2. Hydromorphology and typology

The physical structure and hydrological regime of water bodies, largely determines the nature, structure and function of aquatic, wetland and riparian biotic ecosystems (Gorman & Karr, 1978; Poff & Ward, 1989; Mitsch & Gosselink, 1993). Hydromorphology is determined primarily by climate, catchment topography and geology. It is of major importance for water body typology. Waterbody type is required to be defined for each water body under Article 5 (Annex II) of the WFD. Factors effecting change in hydromorphology are required to be considered in the monitoring required under Article 8 of the WFD, as a supporting element to water body classifications as described in Annex V. Modelling of hydromorphology is implicit in hydrological models, since much of hydrological modelling is concerned with predicting the consequences of change in land or water use in the catchment, within the channel, or indeed in climate.

3.2.1. Rivers

Alteration of flow regimes in rivers can clearly affect biotic communities, and hence classification of ecological status. While it is possible to estimate ecological optima for some individual biotic components, this is not feasible for all organisms. The underlying philosophy of the WFD that maintenance of natural hydrologic regimes is the primary requirement to support *high* status of ecological diversity is explicit in the normative definitions contained in Annex V of the WFD. Alteration to the range of flows within a river may compromise attainment of *good* status and, in particular, impact on floodplain processes, riparian vegetation and integrity of associated wetlands. Hydromophological management, and models, for rivers need, therefore, to incorporate a wider dimension than the river channel alone. In addition, river habitats not only depend on floodplain processes, but habitat diversity of natural floodplains also depend river dynamics (Richards *et al.*, 2002). As such, characterisation of the catchment required under Article 5 of the WFD would usefully consider fluvial architecture (Miall, 1985) and floodplain dynamics (Nanson & Croke, 1992). While there is not a long history relating ecosystem integrity to flow regimes and, because variation of flows are so important for that, commonly used statistical tools can be inappropriate (Richter *et al.* 1996) They do not, for example, reflect extreme events well or deal effectively with issues of replication for comparative analysis within sites (Stewart-Oaten *et al*., 1986, 1992). Some recent developments of models that appear highly applicable for assessment of hydromorphology of rivers may be highly relevant to the implementation of the WFD.

Model simulation of changes in river morphology (Howard, 1992; Murray & Paola, 1997) that provide insight to expected changes in the medium-long term may not be considered applicable to the immediate time scale of WFD implementation; but may be important in the longer-time scale and should not be discounted. The time scale of natural processes are not always conveniently matched with those of political immediacy**.** Time-scales (years to decades) that clearly do relate to contemporary management are those that affect channel patch dynamics (Richards *et al*., 2002) and models of alterations to river hydrology using pre- and after-impact data from recent history (Richter *et al*., 1996). For example, river regulation by channelisation or flood control increases prevalence of terrestrial vegetation from reduced turnover of fluvial landscapes and are highly applicable to model development and use (Richards *et al*., 2002). Paramount in the development of these models may be the prediction and understanding of the effect of water pulses along a channel, and quantification and assessment of effect of high (flood) and low (drought) flows. Models that simulate patterns of geomorphology or habitat succession and replacement are valuable tools for river and floodplain assessment and management. At the floodplain scale, developments in remote sensing technology and incorporation within GIS (e.g. Mertes, 2002; Winterbottom & Gilvear, 1997; Johnson, 2000) also provide valuable modelling tools for characterisation and prediction of impacts or restoration strategies.

Modelling of processes within the appropriate scale of the reach that relate to geomorphological structure and associated riparian (Richards *et al*., 2002; Cordes *et al*., 1997) and in-stream habitats are important recent developments. Simple models that relate biotic communities to characterisation of mesohabitat structure (Harper *et al*., 1995; Armitage *et al*., 1995) have high potential for cost-effective assessment of effects of physical changes in not only rivers but also lakes (White and Irvine, 2003) and transitional waters. Future developments will likely be the coupling of hydrological models with those of ecological components such as floodplain plant successions (Richards *et al*., 2002), and in stream biota. Developments useful for prediction of fish communities are described in section 3.4.3., *'Habitat (fish) models'*.

Richter *et al*. (1996) proposed a method for assessing hydrological alterations in river channels using a multimetric approach with Indicators of Hydrological Alteration (IHA). The methods used 32 estimates of mean tendency and associated statistics of dispersion (e.g. timing, coefficient of variation) to characterise inter and intra-annual flow regimes. The metrics were divided into five groups that defined the:

- magnitude of flow;
- timing of occurrence of key water condition;
- frequency of occurrence of conditions;
- duration of water condition; and
- rate of change of water conditions.

All metrics were considered to be of potential biological relevance. The IHA method compares hydrological condition within a single site before and after disturbance. While this permits estimation of the magnitude of impact, it does not provide a firm basis for causal links. The method can, however, enable comparisons between different reaches up and below stream of an impact based on modelling that can fill in data gaps or simulate pre-or post-impact conditions (Alley & Burns, 1983; Linsley *et al*., 1982; Paller *et al*,. 1992).

Concepts and models important for eco-geomorphology of rivers and floodplains are discussed further in Richards *et al*. (2002) and, for assessment of hydrologic alteration using hydromorphological metrics, by Richter *et al*. (1996) and Richter *et al.* (1998). Further progress with these models have benefit for catchment characterisation and water body classification required under Article 5 of the WFD and, through e.g. scenarios for restoration, programmes of measures, required under Article 11.

Water level (hydraulic) models

Models based on hydraulic equations, and used with hydrological inflow series and channel cross-sectional data, can predict water levels, flow velocities and scour. Models that predict water levels are often associated with engineering design projects, and relate to changes of a single dimension of depth (e.g. SWMM, HEC-RAS). Their usefulness in relation to the WFD relates to their ability to model and design/manage water flow conditions at specific locations or in specific reaches. For example, mean values and possible ranges of water depth and flow velocity may be critical for certain habitats/species. Measurement of these variables at suitable intervals, even over long time periods, may not give realistic ranges of these variables, e.g. corresponding to infrequent floods or droughts and modelling. Prediction can only be made using low-probability (long return period) flood/drought magnitudes inferred from a frequency analysis and hydraulic model. This work requires water level monitoring equipment, which is becoming increasingly economical to install and operate, and is re-deployable. It is also frequently used for high temporal resolution sampling and design of flow-proportional sampling regimes.

Low flow estimation models

Gridded data sets of hydrologically-relevant variables allows generation of flow parameters for ungauged sites. In the UK, Micro Low Flows (MLF) was the first software product of this type to be made available for the Environment Agency, the Scottish Environment Protection Agency and the Northern Ireland Environment and Heritage Service (Young *et al*., 2000). Low Flows 2000 is the successor to MLF and, in the UK, benefits from "longer periods of record, new records, updated climatic data sets and new approaches to regionalisation" (Holmes and Young, 2002). While much of its use will still be focused on deriving low flow statistics for ungauged sites, it will generate the ordinates of a full flow duration curve on either an annual or a monthly basis. It provides a development of assessing anthropogenic impacts on flow, introduced in MLF. It is presented as a catchment management support tool, since flow alterations such as irrigation abstractions or effluent discharges impact on the use/availability of water elsewhere in a catchment. Groundwater fed flow can clearly be important for stream ecology. An analytical solution within Micro Low Flows enables the estimation of the influence of groundwater abstraction on low flows. Recent work funded by the UK Environment Agency is developing a methodology to summarise qualitative and semi-quantitative macroinvertebrate response to flow variations in chalk streams, which could be developed to identify relevant hydrological and ecological thresholds. This work forms part of a European project (LIFE) that is investigating efficiency of policies for the prevention and control of diffuse pollution to surface water, and coordinated by WRc, UK.

Recommendations: Low flows models should be further investigated for applicability for the estimation of impact on ecological indicators and reference conditions, and to develop flow duration curves to be estimated for ungauged sites.

Flow regime alteration models

Many approaches to the assessment of hydrological alterations have been attempted and are commonly incorporated as rainfall-runoff model in many catchment models. Where there have been hydrological distortions to flow regime, a model developed in Scotland for WFD implementation, the Dundee Hydrological Regime Assessment Method (DHRAM) (Black *et al.*, 2000) may be useful for application in Ireland. The method is recommended as a screening tool to identify heavily distorted hydrology that risk affecting ecological status. The tool has been tested in many parts of Scotland where, *inter alia*, hydro schemes affect many upland river systems, but is applicable to other single or combined impacts on river flow regimes or lake levels. One strength of DHRAM is that it assesses a comprehensive range of distortions to hydrological regimes (encompassing magnitudes of monthly mean and *n*-day extreme flows, flow seasonality, frequency and duration of high and low flow pulses, and rate and frequency of flow changes). Because of this generality it is considered applicable to Ireland, but does require a means to generate daily synthetic river flow (or lake level) data on a routine basis for ungauged sites; a demand which can be met by a tool such as Low Flows 2000 in conjunction with measured daily flows from an unmodified gauged analogue site.

European standardisation for river classification and the River Habitat Survey

Prompted by the requirements of the WFD, the Standardisation of River Classifications programme (STAR; http://www.eu-star.at/frameset.htm) is an EU funded project seeking to develop standard methods for implementation of both biological and hydromorphological assessments. Progress in relation to developing a European standard approach, ultimately leading to the adoption of CEN standard, reported by Buffagni and Erba (2002), has shown four European countries with relatively well-developed national programmes for the hydromorphological assessment of rivers.

These are:

- Austria Nation-wide method
- France SEQ Physique
- Germany LAWA-vor-Ort
- UK River Habitat Survey (RHS)

Owing to variations in input data and different methods for calculating levels of morphological impairment, these schemes did not produce directly comparable results. Ultimately, therefore, the RHS approach was used throughout the consortium of European partners.

The River Habitat Survey (RHS) has been developed by the Environment Agency for England & Wales as a means of using physical data to predict habitat quality (Raven *et al*, 1997; Fox *et al.*, 1998), although it continues to undergo further refinement. It is, however, highly applicable to the assessment of hydromorphological elements that support the biological ones outlined in Annex V of the WFD. One particularly useful element of RHS is the assessment of bank and channel modification by a straightforward scoring system (see further discussion in *River Habitat Survey* in section 3.4). The system is based around a Great Britain and Northern Ireland reference database of more than 5000 sites (Raven *et al.*, 2000), and would be applicable to many Irish rivers. The U.K. database could be extended to Ireland through a collaborative arrangement that could, lead eventually to a comprehensive database that covered the whole of Ecoregions 17 and 18 defined in Annex XI of the WFD.

Existing hydromorphological data in Ireland.

Regulated drainage occurs in over 50% of catchments in the Republic of Ireland. Between 1945 and 1995 the Office of Public Works completed 34 arterial drainage schemes on river catchments. It holds detailed information on the morphology of rivers pre- and post-drainage, together with data for schemes not implemented. It is responsible for the maintenance of over 11,500 km of channel, more than 700 km of embankment and many structures such as bridges, sluices and pumping stations.

Recommendations: Hydromorphological modelling techniques applicable to the WFD require further development. There is, however, clear potential for the extensive current and historical data of the Irish OPW to be “mined” in order to develop a system similar to that of the IHA. A collaborative arrangement with the Environment Agency for England & Wales for development of RHS for assessing hydromorphology in Ireland could be useful for WFD implementation in both jurisdictions.

3.2.2. Lakes

There are many types of predictive models for lake systems. The term 'predictive model' is taken to indicate such models where one to a few important y-variables are predicted from a few x-variables that can be obtained easily from standard topographic maps or from standard lake monitoring programmes. Of particular importance with respect to the WFD, Håkanson and Peters (1995) discuss the use of models in which simple, readily obtainable variables accessed from maps (lake catchment area maps [geology, soils, vegetation, land use], climatological maps, lake bathymetric maps) are used as x-variables to predict certain chemical 'state variables', such as mean lake concentration of total-P, water colour and pH. These, in turn, are used in other models to predict key ecological and biological state variables that are linked to important functional groups or critical ecological parameters. Furthermore, ecological state variables can be used to derive a lake index that expresses the status of the given system. Accurate information on lake morphology is, however, vital in order to predict effects on lake function from alterations in delivery rates of material from the catchment. The application of models can be useful for assessment of the hydromorphological quality elements for lakes listed in Annex V of the WFD (Table 3.1.).

Table 3.1. Recommended hydromorphological elements of lakes to be considered in implementation of the WFD.

Hydrological regime	Morphological conditions
Quantity and dynamics of flow	Lake depth variation
Water level	Quantity and structure of the substrate
Residence time	Structure and condition of the shore zone
Connection to groundwaters	

Quantity and dynamics of flow

The Håkanson and Peters (1995; Chapter 11) dataset from 95 Swedish lakes contains calculated estimates of water discharge (Q, in $m^3\ a^{-1}$). Q has been determined from ADA (the lake catchment area in km^2) and maps of specific runoff (SR in $m^3\ km^{-2}\ a^{-1}$; i.e. Q = ADA*SR) show a simple linear regression between Q and ADA. It is evident that SR does not vary a great deal among these 95 water bodies and that Q may be predicted rather well from ADA. It is also evident that this is a rather rough estimate, since SR is a map constant, and that Q in reality varies with precipitation, season of the year, vegetation cover, geology and soil type. Nevertheless, regression analysis between Q and ADA may prove useful for application to Irish lakes. Comparison of theoretical, from run-off-precipitation estimates, and measured Q can provide useful insight to loss to groundwater, particularly in karst and semi-karst areas.

The overall rate of throughflow of a lake is susceptible to modification through alteration of the hydrology of the rivers or streams that feed it. The Dundee Hydrological Regime Assessment Method (DHRAM) incorporates a method to quantify the degree to which the flow regime of a river, or the level regime of a lake, expressed in terms of variables that are significant to ecology, departs from the natural condition (Black *et al*., 2000a, b).

Water level

The DHRAM method incorporates a method for calculating anthropogenic alteration of water levels in Scottish lochs. This generates one of five classes, ranging from ‘unimpacted condition’ to ‘severely impacted condition’. Central to the procedure is the concept of a natural neighbour (analogue site) which is used as a baseline against which to measure alteration wherever direct observations of anthropogenic impact are lacking. Along with the REGCEL (Hellsten *et al.,* 2002) model, this method has been applied to analyse impact of water level fluctuation in regulated Lake Vaggatem, Finland (Hellsten *et al*., 2002). Both methods provided a simple way to analyse environmental changes without the need for time-consuming fieldwork. The main difference between the REGCEL and DHRAM models is that the REGCEL model emphasises critical water levels which, according to empirical evidence or expert judgement, cause harmful impacts on e.g. littoral vegetation, zoobenthos and fish. The REGCEL model also takes into account site-specific factors that affect sensitivity of the system to hydromorphological pressures. This water level analysis model developed by the Finnish Environment Institute calculates more than 30 parameters of daily water level values, is coded by Visual Basic and uses an Excel program. The DHRAM model is based on the assumption that the alteration is always harmful, without estimating the adaptability of ecosystems to change (Hellsten *et al.*, 2002). These approaches appear appropriate for modelling the impacts of water level changes in Irish lakes.

Residence time

Residence time, T (also known as lake water retention time or turnover time) is a crucial concept in limnology. It is defined as the ratio of the lake volume, V (capacity), and the water discharge, Q (the latter is often expressed as the mean annual runoff, in which case T is the theoretical residence time): This definition assumes the entire volume of the lake is hydraulically active, which may not always be the case.

In situations where the mean annual inflow to a lake is unknown, R may be estimated using a water budget relationship:

$$E = P + I + U - R \pm S \qquad \text{(equation 3.1)}$$

Where:
E = evapotranspiration from lake surface;
P = total precipitation onto lake surface;
I = direct surface inflow from surrounding lands;
U = Underground outflow (or inflow);
R = catchment runoff; and
S = change in storage (both surface and sub-surface).

If surface inflow, underground outflow and storage changes are assumed to be negligible, then:

$$R = P - E \qquad \text{(equation 3.2)}$$

R may, therefore, be estimated numerically from data readily obtainable from climatological maps. Use of water budgets need, however, to incorporate the realisation of inherent uncertainty in the measurement of some of these quantities. Large lakes/reservoirs influence the local climate and on-shore measurements of, for example, precipitation and potential evaporation may not give accurate estimates of these fluxes over the lake.

Lake volume, V, is often not known since, in many cases, bathymetric maps (and therefore hypsographic curves) are not available. In this event, to estimate residence time, it is necessary to predict lake volume. Håkanson (1997), following the rationale for a new approach to defining lake water retention rate (Figure 2.38 of Håkanson and Peters, 1995), has suggested the following predictive relationship between V (km^3) and variables that can be readily determined from topographic maps:

$$\log(1000*V) = 0.134 + 1.224*\log(A) + 0.332*\log(RDA) \quad \text{(equation 3.3)}$$

Where: A = lake area (km^2)

$RDA = dh / (\sqrt{ADA})$

And: dh = altitudinal range of catchment area (m)

ADA = drainage area (km^2)

The above relationship would, however, require verification and validation for Irish standing waters.

An early example of the development of predictive limnology was the work of Gorham (1958) who used the Murray and Pullar (1910) bathymetric data from a total survey of 562 Scottish lochs. Gorham (1958) examined the following inter-relationships between drainage area, lake surface area, length, mean breadth, mean depth and maximum depth for 262 rock basins and 137 basins lying in or dammed by glacial drift:

- Length and mean breadth;
- Drainage area and lake area;
- Mean depth and lake area;
- Maximum depth and mean depth; and

- Replacement time (i.e. residence time) and lake area

For example, a relationship (r = 0.68) was derived between mean depth and lake area for rock basin lakes but for drift basins, the relationship was insignificant (r = 0.24). Whilst the Republic of Ireland does not have a similar wealth of lake bathymetrical data to Scotland, it nevertheless has some (e.g. Irvine *et al*., 2001; Horkan & Toner, 1984; Bowman, 1985; Allott, 1990). Collation and simple regression analysis of the available data would be useful to explore predictive equations for e.g. lake volume, as described by Håkanson (1997). It is, however, likely that modelling of bathymetry is more feasible for lakes in catchments of high relief than shallow relief. For many Irish midland lakes, knowledge of surrounding topography may not be a reliable indicator of lake volume or shape, but this requires further study

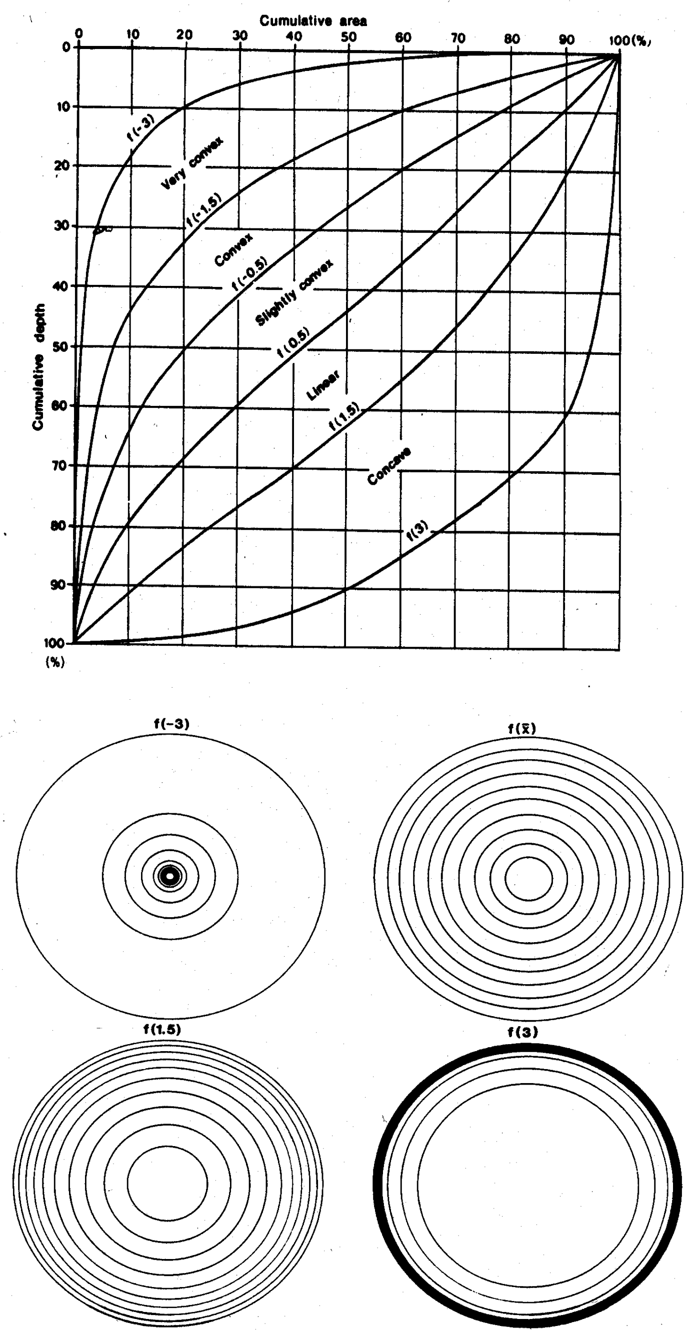
Whether or not a lake stratifies in the summer months has a significant impact on residence time, since hypolimnetic waters will be essentially stagnant during such conditions whereas the waters of the epilimnion will be subject to exchange (Figure 2.38 of Håkanson and Peters, 1995). Allott (1990), in a simple ordination of 35 British and Irish lakes by plotting maximum depth (x) against length (y), discriminated stratifying from non-stratifying lakes. This simple approach merits further consideration for estimations of residence times.

Lake depth variation

In order to determine lake depth variation, information on the basin form must be known. While variables such as mean and maximum depth might be predicted as described above, lake depth variation requires bathymetric data. While it might be possible to broadly predict the form (see Håkanson, 1981) of an unsurveyed lake from survey data of neighbouring lakes of the same origin in similar geological terrain, this will not necessarily provide a good representation of lake depth variation. While actual survey is, therefore, needed to map variations in depth, use of models that interpolate between measured locations can be useful. Such an approach was used by Irvine et al (2001) in the determination of depths of a number of Irish lakes.

Hypsographic curves (Figure 3.2.) can assist greatly with determination of internal lake structure, and e.g. influence of prevailing winds on fetch, likelihood to stratify and importance of the littoral in the overall ecology of the lake. While good hypsographs may require field assessment of bathymetry, once established they can be highly useful in assessment of response of lake nutrient and biotic regimes to impacts a)

b)



Lake form	**Class limits**
Very convex	f (-3) to f (-1.5)
Convex	f (-1.5) to f (-0.5)
Slightly convex	f (-0.5) to f (0.5)
Linear	f (0.5) to f (1.5)
Concave	f (1.5) to f (3)

Figure 3.2. a) Terminology and class limits for the classification system of lake forms. b) Schematic bathymetrical interpretation of four statistical lake forms (After Håkanson, 1981).

Recommendations: The REGCEL and DHRAM, and methodology to model residence times approaches could be usefully adopted for assessing hydrological impacts to lakes and their ecology in Ireland. Hypsographic curves for Irish lakes should be compiled and this information applied for estimation of residence time and lake physical structure. Simple modelling techniques to estimate mean depth and likelihood of stratification of Irish lakes need further exploration.

Connection with groundwaters

The degree of connectivity between lake and groundwaters is influenced most strongly by the permeability of the solid and/or drift geology in which the lake basin has developed, and to a lesser degree by basin form. An important characteristic is the ratio of groundwater inflow or outflow to total inflow or outflow, on the basis of which lakes can be divided into two groups; those that are groundwater dominated and those that are surface water dominated. Groundwater-lake relationships may be explored by direct measurements of the seepage flux through the bottom sediments, by tracer experiments, through study of the water balance (see above) or by using Darcy's Law (Annex 1). In general, the permeability characteristics of the soils surrounding a lake are much more important in determining the degree of hydraulic connection between lake and groundwater than are the thickness, permeability and distribution of sediment within the lake. Vanek (1985) presented vertical section models to show seepage pattern at a lake margin. This approach merits further investigation. Sometimes a relatively thin layer of low hydraulic conductivity can be a major factor in controlling such seepage fluxes. In modelling such cases, the role of unsaturated soil suction has often been neglected and can be very influential (Osman & Bruen, 2002).

The link with groundwaters is also important for rivers and wetlands. Simple modelling approaches can help quantify the influence of groundwater on wetlands and impact on wetland vegetation caused by e.g abstraction and channelisation. In general, groundwater influence on wetlands can be absolute (such as in the case of turloughs) or as a minor factor in sustaining wetland characteristics. Groundwater abstraction can lead to delayed impact on wetland integrity.

Results of work on impact of water table on plant communities in wet grasslands (e.g. Gowing *et al*., 2002) has quantified relationships between species and hydrological drivers and has helped develop data interpretation and monitoring strategies for wet grassland management. Hydrological models of Youngs *et al*. (1989), Young (1994) and Gowing *et al*. (1998) were used to simulate water-table behaviour as a surrogate for both root-zone water potential and soil aeration. Threshold values of waterlogging, based on Sieben (1965), were estimated across a range of sites and related to botanical community data. The work covered all the major floodplain grassland communities of conservation interest in England and Wales. Each showed a characteristic water regime.

A more detailed discussion of groundwater modelling comprises Chapter 5 of this report.

Quantity and structure of the substrate

Sedimentation rates in lakes can increase owing to pressures in the catchment and is of extreme importance for the estimation of mass-balance of lakes (section 3.3.7), it is also a fundamental phenomenon in all lakes. Håkanson and Peters (1995) provide a model of gross sedimentation based only on x-variables that can be read from standard maps (e.g. Ordnance Survey Maps) of the catchment area and the lake. Some important working hypotheses in the development of this model were:

- No single factor is likely to explain statistically and/or causally the great variability in net or gross sedimentation that exists among lakes;
- It is improbable that a single lake sedimentation model can be used for all lakes;
- No meaningful models based on 'constants' from topographical, bathymetric or soil maps could be developed without a characteristic value of lake sedimentation;
- A dynamic approach began with a mass balance equation using input data on water discharge, concentration of suspended matter and, possibly, total-P in the tributaries and in the lake;
- Allochthonous (i.e. catchment derived) input is assumed to be affected by catchment area, drainage area zonation (location of lakes, mires, etc.) and the geological characteristics of the drainage area; and

- Autochthonous (i.e. within lake derived) production and resuspension are assumed to be linked to the size and form of the lake.

Topography and bathymetry of lakes

It is important that topographic and bathymetric maps of lakes are reliable, so that the input data for models are similarly reliable. Håkanson and Peters (1995) examined linear correlations (r values) between 53 'constants' derived from drainage area and bathymetric maps, water chemistry and the measured values of gross sedimentation. The volume development (or the form factor, $V_d = 3*D_m/D_{max}$, where D_m = mean depth and D_{max} = maximum depth) was found to be the characteristic most strongly correlated to gross sedimentation ($r = 0.51$). The empirical relationship between the volume development and the rate of sedimentation showed that the residual scatter around the linear regression was considerable ($r^2 = 0.26$) and that the rate of gross sedimentation increased with Vd. The data suggest that (at least for the lakes studied), there is a significant positive relationship between Vd and the rate of gross sedimentation. Although Vd does not explain all the variability in gross sedimentation between the lakes, the regression explained 25-26% of the variability in gross sedimentation among the lakes studied with the form factor (which reflects both form and size). Stepwise multiple regression analysis used by Håkanson and Peters (1995) highlighted the importance of the relative depth of a lake (D_{rel}). This represents form and size elements of a lake and is conceptually linked to resuspension:

$$D_{rel} = (D_{max}*\sqrt{\pi})/(20*\sqrt{area}) \qquad \text{(equation 3.4)}$$

D_{rel}, together with five other lake characteristics, yielded a model that explained 78% of the variability in (the logarithm of) gross sedimentation among the 25 lakes studied. This iteration of the model may, however, be too complex and cumbersome (further research is needed in this respect) for implementation of the WFD. It should, therefore, be noted that D_{rel} alone explained 45% of the variability in gross sedimentation rates in the lakes studied (Håkanson, 2003).

Altered sedimentation in impoundments has attracted a lot of attention and modelling effort because of the impact on storage capacity and pollutant load. Considerations of sediment load to impoundments are, *de facto,* site specific issues. Modelling of sediment transport in reservoirs range from a simple 1-dimensional approach for the estimation of net longitudinal transport, 2-dimensional for sediment vertical profiles or 3-dimensional in relation to e.g. sedimentation in water intake. While the traditional need for modelling of sedimentation in reservoirs has related mainly to engineering operational capacity, under the WFD there could arise a need to also relate this to impact on ecological potential for heavily modified water bodies (section 3.2.4). In Ireland, however, impact from increased algae populations in standing waters is likely to be of greater concern, and can be modelled as for lakes (section 3.4.3, *Periphyton*).

Structure and condition of the shore zone

Shoreline habitat measurement is important for identifying possible causes of ecological impact because many lakes are impacted by development on or near the shore zone. Shorezone development through pressures such as housing or industry can have a disproportionate impact on nutrient loadings compared with more distant parts of the catchment.

The United States Environmental Protection Agency (USEPA) has developed comprehensive monitoring, bioassessment and biocriteria programmes for lakes and reservoirs. Two schemes of particular potential for application to the WFD are: (1) Surface Waters Field Operations Manual for Lakes (FOML), which provides protocols for data collection on water quality, ecological variables and physical structure, and was developed as part of the national Environmental Monitoring and Assessment Program (EMAP) (Baker *et al*., 1997); and (2) the Habitat Measurement Programme (HMP), developed for the classification of lakes and effects on biological integrity of anthropogenic disturbances and exposure (USEPA, 1998).

The EMAP programme through the FOML has developed an extensive shorezone and littoral survey methodology to characterise riparian, shoreline and littoral habitat. Survey time is prescribed as late summer when vegetation is at its annual maximum. The riparian characterisation consists of estimates of dominance of vegetation in canopy, understorey, and groundcover; substrate type; bank angle; and dominance of human features (e.g. buildings, industry, cultivation). Littoral characterisation is done at a 10 m distance from shore and includes depth, surface film, substrate, macrophyte cover, fish cover, and a summary habitat classification. The shore of each lake is surveyed at 10 sites, and the frequency of disturbance is estimated for each lake from the survey data (Figure 3.3). Assessment of medium-scale 'mesohabitats' in lakes can provide a useful tool for ecological classification and monitoring (White and Irvine, 2003).

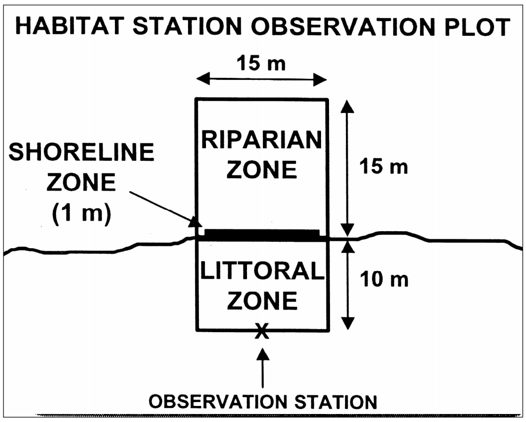


Figure 3.3. Sketch map showing the dimensions of observation plot at each station of the EMAP scheme

The HMP programme (Table 3.2.) offers a simplification of the EMAP FOML protocols. In this scheme, shore zone measurements are means of the littoral and shore zone habitat metric values. The shore zone and littoral cover measurements are expressed as the mean of the values of all transects. The human influence measurements are based on presence or absence observations within the transects. These measurements are weighted, with each present observation receiving a score of 1 and each "adjacent" observation receiving a score of 1/2. The human influence score in each category is the mean of all transects. It is in the range of 0-1, with 0 reflecting no influence and 1 indicating that the influence (e.g., buildings) was found in every transect (USEPA, 1998).

Bragg *et al*. (2003) reviewed existing practice elsewhere in the world, but found no comparable systems currently being used for the systematic appraisal of shoreline condition required by the WFD. On-going research commissioned by the Scottish Environment Protection Agency (SEPA) (D. Corbelli, *pers com)* is considering the application of remote sensing techniques for the appraisal of pressures and impacts and in the generation of suitable measurement metrics. Bragg *et al*. (2003) suggested an appropriate way forward would be to develop a lake habitat assessment scheme based on many of the metrics collected from the FOML, but using a Habitat Modification Score (HMS) analogous to the developments being made in the River Habitat Survey (c.f. Raven *et al.,* 1997). However, a comprehensive testing and validation exercise would be required before such a scheme could be recommended for implementation.

Table 3.2. Lakeshore habitat measurements and metrics (USEPA 1998).

Habitat Measurement	**Mean % Cover**	**Indicator**
Bank Measurement - Rocky (%) - Soil (%) - Vegetation (%) - Other (%)	Mean % cover from shorezone habitat transects	Bank stability
Bank Erosion (0 – 4)	0 = none; 4 = severe erosion	
Riparian Vegetation Measurements - Canopy (% cover) - Understorey (% cover) - Ground Cover (% cover)		Disturbance
Human Influence Measurements Buildings - In-lake structures - Roads, railroads - Agriculture - Lawn - Dump or landfill	Influence score (mean score of transects) Presence / absence	Human influence

Recommendations: Predictive models based on data readily derived from maps, and following Håkanson and Peters, (1995) should be explored for Irish lakes in order to model quantity and structure of the substrate. Further development and testing of mesohabitat assessment and models for lakes could provide a cost-effective aid to monitoring.

3.2.3. Transitional waters

Classification

Owing to changing river flows, tidal dynamics and sediment distributions, many estuaries and transitional waters may never reach steady-state. Because of the interaction of many variables no two estuaries are alike and it is often difficult to separate observation of general principles from unique features (Dyer, 1997). In order to compare estuaries, various classifications have been devised based usually on topography, river flows and tidal action. Wind and waves may also be significant. A topographic classification by Pritchard (1952) divided estuaries into three groups: coastal plain estuaries, fjords and bar-built estuaries:

- *Coastal plain estuaries* are generally restricted to temperate latitudes; river sediment load is relatively small and river flow generally small compared with the tidal prism. Most Irish estuaries are of this type.
- *Fjords* generally have rocky floors and river discharges are small compared to the fjord volume but may be large compared with the tidal prism. Their occurrence is generally restricted to high mountainous regions at high latitudes. Killary Harbour is the only Irish fjord.
- *Bar-built estuaries* have a characteristic bar across their mouths. For this bar to be fully developed, the tidal range must be relatively small and there must be large volumes of sediment available. These estuaries are often only a few meters deep and often have extensive lagoons and shallow waterways just inside the mouth. River flows are seasonally variable with large volumes of riverborne sediment at flood times. During flood the bar may be swept away completely, but quickly re-established during low flows. Bar-built estuaries are generally found in tropical areas.

Cameron and Pritchard (1963) classified estuaries by their stratification and characteristics of salinity distributions, which lead to a better understanding of how circulation of water in estuaries is maintained. They defined four main estuarine types: highly stratified or salt wedge, fjords, partially mixed and homogeneous. Most Irish estuaries are of the partially mixed/homogeneous types. There is obviously some correspondence between the results of classification on topographical and salinity structures; it is clear though that the limits of estuarine type are never well defined. Simmons (1955) found that when the flow ratio (ratio of river flow per tidal cycle to the tidal prism) is greater than 1.0 the estuary is highly stratified. When the flow ratio is about 0.25 the estuary is partially mixed and when less than 0.1 the estuary is well mixed. This approach is, however, approximate as estuarine width and depth also influence mixing. For example, the Mersey Estuary has a flow ratio of 0.01 and yet is partially mixed. Estuarine type may also show variation along its length and flow ratios may change dramatically from season to season.

Ippen (1966) discusses the use of a stratification number to assess the mixing in estuaries based on energy computations. Increasing values of the number indicate increasingly well-mixed estuaries, with the converse for low values. The stratification number depends on breadth and width of the estuary and, hence, similar river discharges and tidal dynamics in estuaries of different dimensions will produce different stratification numbers. The method requires accurate measurements of tidal elevations at several positions along an estuary and knowledge of river flows.

Hansen and Rattray (1966) developed an estuarine classification based on dimensionless parameters of a) stratification parameter and b) circulation. This approach requires measurements of salinity and velocities and classifies four hydromorphological types:

- *Type1* Net flow is seaward at all depths and upstream salt transport is by diffusion
- *Type 2* Flow reversal occurs with depth and to the partially mixed estuary
- *Type 3* The salt flow is primarily advective
- *Type 4* Stratification is intense and corresponds to a salt wedge type estuary

Estuaries are often classified according to their residence or flushing times. These parameters provide *inter alia* an indication of the assimilative capacity of estuaries and are particularly useful in make intercomparisons between different estuaries. Flushing times may range from several hours to weeks or months. Numerous methods have been developed to compute flushing times and residence times such as the methodologies described by Hartnett *et al.* (2003), Sandford *et al.* (1992) and

Takeoka (1984). The methodologies used to compute these parameters range from using gross estuary characteristics to using detailed hydrodynamic and solute transport models.

Morphology

Estuarine sediments are transported, as in streams, as bed load and suspended material. Erosion and deposition alternate with tidal motion, but net transport is governed by average velocities over a tidal cycle. According to Ippen (1966) the following general conclusions regarding sediment transports are:

- Sediments settling to the bottom will on average be transported upstream and not downstream
- Sediments will accumulate near the ends of the intrusion zone and form shoals
- The intensity of shoaling will be most extreme near the end of the intrusion zone for stratified estuaries and will be more dispersed in well mixed estuaries.
- Anthropogenic impact may alter natural patterns of hydromorphology by:
  The major portion of sediments introduced into an estuary from whatever source during normal conditions will be retained in the estuary. If transportable by the currents the sediments will be deposited near the ends of the saline intrusion.
- Any measures contributing to a shift in the regime towards stratification will cause increased shoaling. Such measures may be: structures to reduce the tidal flow and prism, diversion of additional freshwater into the estuary, deepening and narrowing the channel.
- Dredging of sediments from channels. This should be accompanied by removal of the sediments from the estuary. Dumping downstream is almost always useless.

Climate Change

Although significant effects of climate change may not be felt at the scale of implementation of the WFD it is worth considering some recent findings. Sweeney *et al.* (2003) predicted a mean sea level increase of 0.48m over the next 100 years. The effect this will have on estuaries is to enlarge their vertical and horizontal extent, resulting in the penetration of tides further upstream. These changes in estuary morphology would diminish sediment supply to the coastal zone as the sediment would be retained within the confines of the estuary. Salt marshes and sand dunes provide a variety of habitats for a range of different species. Many of the marsh systems in Ireland provide over-wintering feeding grounds for many species of migratory birds. The loss of these habitats could present major problems for species numbers and diversity.

Energy is supplied to the coast through wind, waves and currents. The level of energy that a location receives depends on e.g. aspect in relation to dominant wave direction, tidal range, water depth and location in relation to the surrounding morphology. Studies conducted on the east coast of Britain predicted that estuaries could migrate landwards at a rate of 10m per year, assuming a sea level rise of 6mm per year (Pethick, 2001). While, man-made modifications at the coast could act to inhibit these migrations, this causes other consideration in relation to impact – natural hydromorphology which will need to be incorporated within implementing the WFD

Anthropogenic Impacts

Invariably man-made coastal structures affect hydrodynamics and morphology to a greater or lesser degree. A major barrage across an estuary will have significant impacts upstream and downstream of its location and minor structures such as gryones will redistribute local sediments. It is impossible to predetermine the impacts of developments without undertaking detailed computer modelling studies of: wave climate, sediment transport and sediment budgets. From such analyses predictions of morphological change are made often at a gross level, but it is often difficult to predict the detail of sediment redistribution post-development. Obviously, the impact on ecology and habitats will vary depending on, for example, if mudflats are flooded or new mudflats are generated.

Recommendations: It is important to be aware that estuaries are continually changing and hence current morphological features should not be considered as permanent. Many naturally occurring morphological changes (including climate change impacts) are slow and may be insignificant during the first phase of implementation of the WFD. Anthropogenic impacts can, however, be significant, sometimes dramatic, over a relatively short time. To quantify such changes it is usually necessary to carry out detailed computer modelling of some or all of: tidal dynamics, wave dynamics, wind dynamics, sediment transport and sediment budgets.

Modelling transitional waters, and estuaries in particular, is generally considered a complex problem. As opposed to lake, river and groundwaters, steady state conditions cannot be applied to simulating water circulation, material transport and chemical, physical, biological and ecological processes. The primary reason why unsteady conditions must be simulated is owing to tidal dynamics. Because of the unsteady nature of this problem, models such as MIKE21, DIVAST and TELEMAC have been developed specifically for transitional/estuarine conditions.

Water quality models have been developed of many transitional and coastal Irish water bodies over the past twenty years and applied to various diverse water bodies such as Dublin Bay, Cork Harbour, Galway Bay, Wexford Harbour, Shannon Estuary, Donegal Bay, Killybegs Harbour, Bantry Bay, Youghal Harbour. Different models and different levels of modelling have been used. Methodology applied has not been uniform. In some studies the transport and dispersion of single nutrients has been simulated, whereas in others complete nutrient cycling have been estimated. There has not been an inter-comparison study carried out to assess the suitability of particular models to Irish conditions; however, most general purpose water quality models can be applied to Irish waters by specifying relevant boundary conditions and discharges.

Mathematical models of tidal waters need to addresses two distinct problems of pollutant discharge: (i) the near-field problem and (ii) the far-field problem. The near-field problem is concerned with delineating the mixing zone local to the discharge source, whereas the far-field problem addresses the spread and fate of the pollutant as it is advected and dispersed by turbulent currents away from the source location. Usually the models utilised to analyse each of these problems are not integrated. The most commonly used near-field model is probably CORMIX. Most hydrological and water-chemistry models that have been developed in the past two decades (such as MIKE 21, DIVAST, and TELEMAC) are concerned with far-field modelling.

The generally shallowness of Irish coastal waters results usually in vertical mixing and flows which can be well-represented by vertically-integrated models. Many coastal waters have also relatively large plan areas with irregular topographic and bathymetric features that, unlike rivers, induce spatial gradients of velocities through the water-body. It is, therefore, usual that hydrodynamic and material transport models of coastal water-bodies are two-dimensional and depth-integrated. Assumptions made in deploying a two-dimensional model need, however, site-specific validation. In some estuaries, lighter freshwaters flow above heavier saline water and, hence, two-dimensional horizontally integrated models or three-dimensional models may be necessary.

Generally speaking, comprehensive two-dimensional water-quality models are built in a modular manner, consisting of the some or all of the following linked modules:

- hydrodynamics that simulates water circulation and predicts water elevations, current speeds and directions. Hydrodynamic modules must be able to include effects of tidal dynamics, wind dynamics and riverine inflows;

- simulation of salinity transport, which is highly dependent on the hydrodynamic module;

- transport of cohesive and non-cohesive sediment , including elements of erosion and deposition, which is also highly dependent on the hydrodynamic module; and

- transport and biochemical interactions between relevant water quality constituents (particular regarding nutrient and heavy metal transport and cycles).

Water circulation patterns are difficult to predict and the complex interactions between constituents can be difficult and computationally expensive to model. Figure 3.4 presents a schematic illustration of the interactions included when modelling nutrients and chlorophyll_*a*. Data requirements and output of simulations of coastal models can generate substantial amounts of data. Most models output data in formats particular to the model. It is worth considering using a standard format such as 'netCDF'(network Common Data Form). NetCDF is an interface for array-oriented data access and a library that provides an implementation of the interface. The netCDF library defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data. The netCDF software was developed at the Unidata Program Center in Boulder, Colorado and is freely available. The netCDF format has been adopted by many users and developers of marine models. Standardisation such as this allows easy interpretation and analysis of model results from any river basin and, hence, makes the model output data more transportable. For each River Basin a suite of model output parameters could be defined and stored in netCDF format; thus modellers/managers working on one River Basin project could easily access and analsye/compare results from other projects. Many tools for visualisation model results and analysing results, such as Matlab and FORTRAN compliers, recognise the net CDF format.

A most important aspect of developing, calibrating and validating models for use in transitional waters is the collection of data. An integrated modelling/data collection programme is necessary to ensure the development of accurate and reliable models. Frequently water quality models are limited by the amount of data available to specify accurate boundary conditions and to validate the models – thereby reducing the confidence in model output.

There has been considerable development over the past ten years of two-dimensional hydrodynamic and water-quality models applied to transitional waters and a comprehensive review is not possible However, many of the most commonly applied models are mostly well-suited to Irish conditions. Experienced modellers should be able to apply these models to Irish transitional waters without major difficulties.

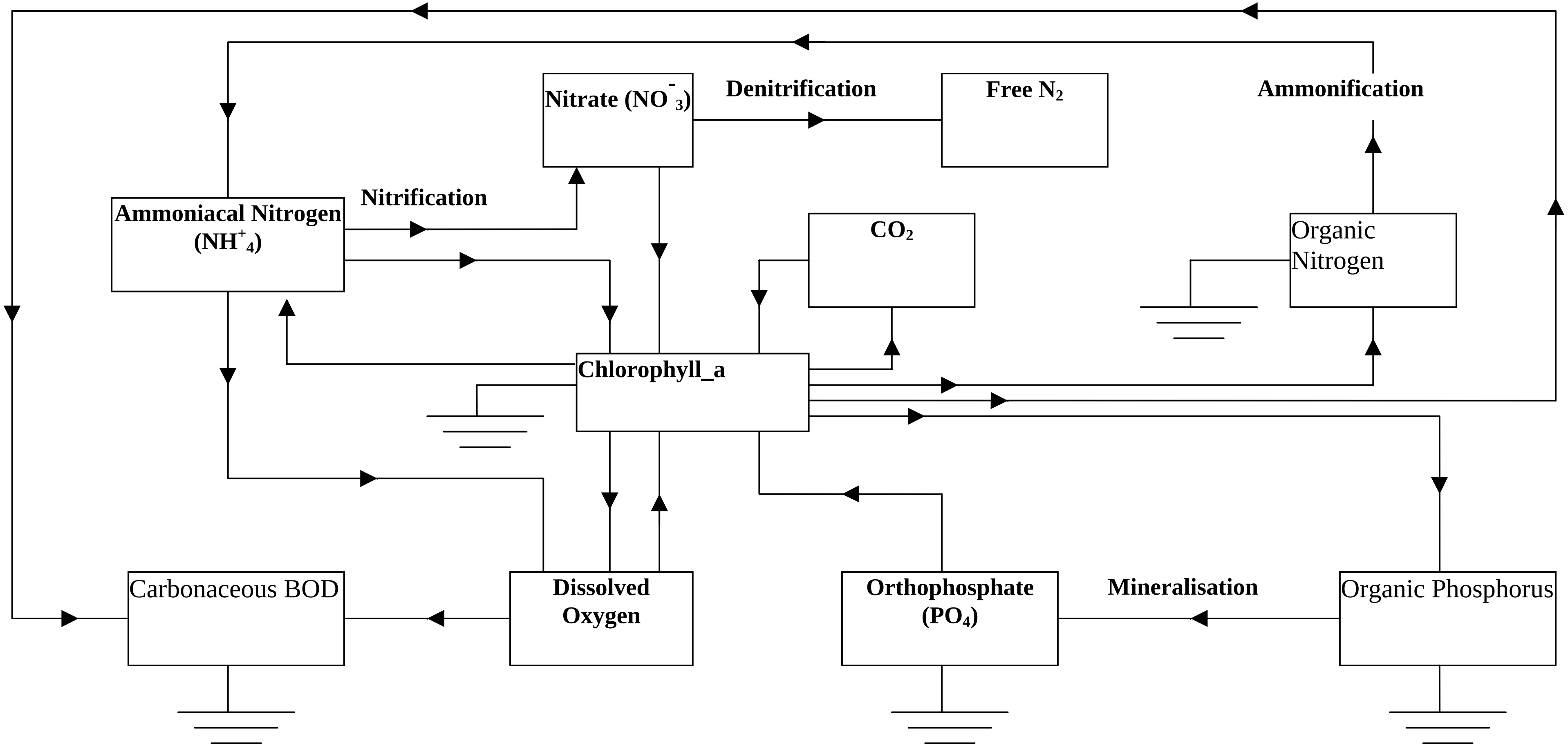


Figure 3.4 – Schematic of Nutrient Modelling

3.2.4. Heavily Modified Water Bodies

The WFD provides for the designation of so-called Heavily Modified Water Bodies (HMWBs), where the requirement to achieve good ecological status is relaxed to allow specifically justified uses of water. HMWBs are water bodies whose character is changed "substantially" by the physical alterations associated with essential water use, and where *good* ecological status cannot reasonably be attained in conjunction with these alterations. A "heavily modified" status means that an unnatural target condition – termed *maximum ecological potential* - may be applied instead of *high ecological status*; for example, the ecological condition of a river reach that has been impounded to create a reservoir may be evaluated against an appropriate reference lake type. The requirement of the WFD is then that the water body must attain *good ecological potential*.

Detailed guidance on identification and designation of HMWBs is given by the WFD Common Implementation Strategy document (CIS, 2002). Candidate HMWBs are selected from those identified as unlikely to achieve *good* ecological status during River Basin District characterisation, on the basis that they have been physically modified (Figure 3.5., Steps 5, 6). For water bodies that are provisionally identified as heavily modified on this basis, the designation tests outlined in Figure 3.6 are applied. Step 1 assesses the potential for restoration of the water body to *good* ecological status without impact on water use. The remaining steps, in essence, constitute a broadly-based feasibility assessment and cost-benefit analysis of the societal function served by the modification.

The evaluation procedures involved are essentially the same as for all water bodies, so that modelling techniques that are appropriate to WFD implementation in general are also relevant here. However, the calibrations of hydromorphological alteration against ecological status that are applied carry particular importance. Critically, Step 5 of Figure 3.5. requires an assessment of the risk of failure to achieve *good* ecological status owing to changes in hydromorphology, whilst Step 1 of Figure 3.6. incorporates definition of the measures required to reverse hydromorphological changes sufficiently to achieve *good* ecological status. Robust calibrations of scales of physical alteration in terms of ecological impact are required. Whilst there could be substantial scope for mathematical modelling in developing these, perhaps from existing models of the relationships between biota and hydromorphology such as those reviewed by Bragg *et al.* (1999), no techniques suitable for direct application in WFD implementation appear to be currently available.

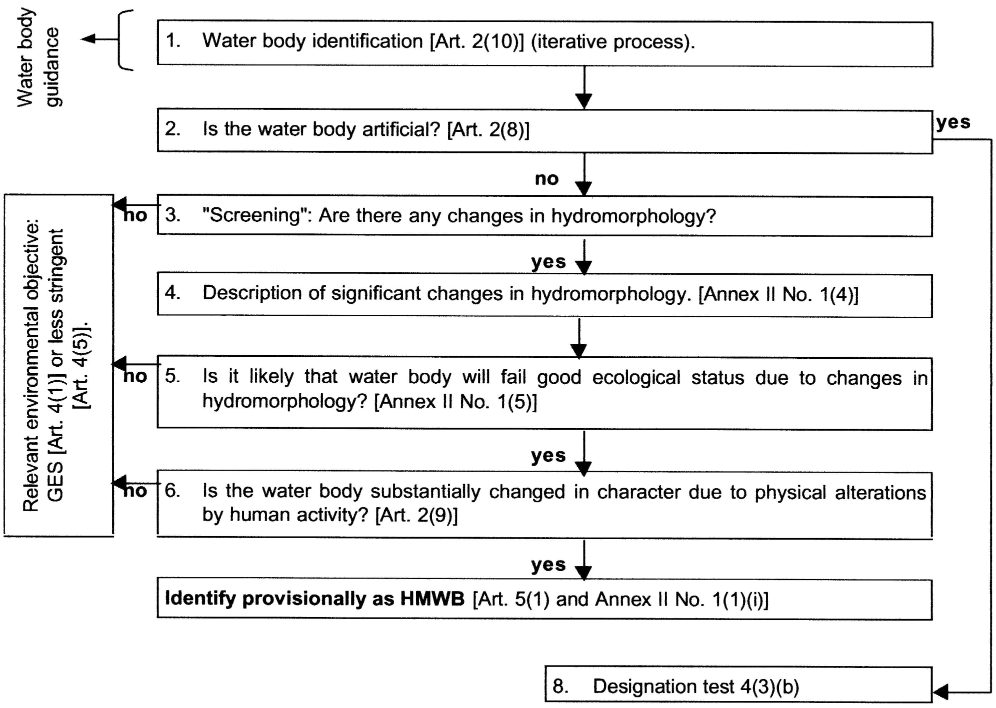


Figure 3.5. Steps leading to the provisional identification of HMWB. From CIS (2002)

HMWB designation trials were carried out across Europe during 2002, and the results were compiled into an "HMWB Identification Toolbox" (CIS 2002). The Toolbox includes examples drawn from all the case studies of approaches to the various steps of HMWB designation. For the Hagmolen-Hegebeck, a typical lowland stream in the Netherlands with significant multiple impacts from agriculture, un-named models were used to forecast separately the hydrological improvements to be anticipated as a result of restoring the stream channel and of reinstating the original catchment area, and, thus, to gain insights into the measures required to achieve *good* ecological potential (Figure 3.6., Step 1). Pre-screening of English rivers for morphological changes (Figure 3.5., Step 3) was based on RHS (River Habitat Survey) and FDMS

(Flood Defence Management System) data in conjunction with published maps, whilst screening for river reaches and lakes with altered hydrological regimes in Scotland was approached using the DHRAM. In Finland, impacts of hydrological change on biology (Figure 3.5, Step 5) was obtained using the REGCEL water level analysis tool.

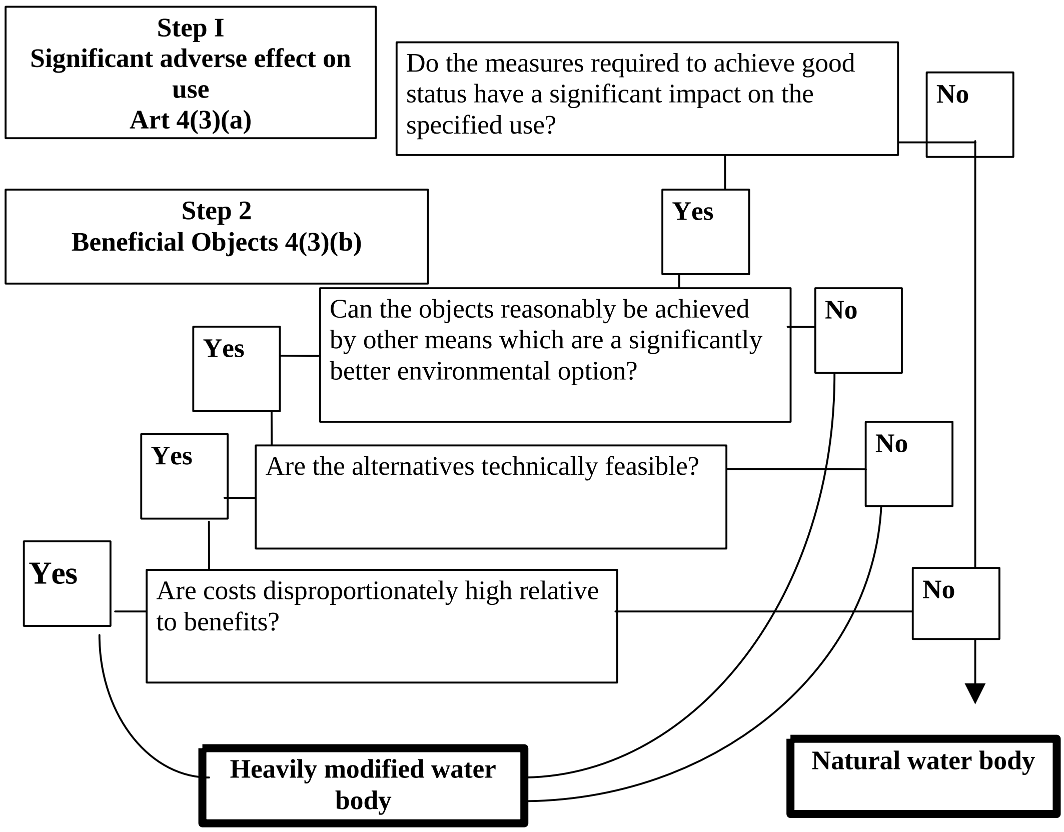


Figure 3.6. Process for designating a Heavily Modified Water Body *(Source: HMWB Project Managers' Paper 8 ver 5e)*

Recommendations: Trial selection and application of Pressure-State and State-Impact models in areas likely to be designated as Heavily Modified Water Bodies. This will allow utility of models to be evaluated in relation to specific situations, and will also allow early recommendations to be reached regarding possible changes in monitoring.

3.3. Pressure-State models

3.3.1. Introduction

Pathways that describe Pressure-State may involve a number of steps and model domains. An example relating to nutrient enrichment in lakes is shown in Figure 3.7. Transport of nutrients to the lake move through a number of potential "gates" that restrict or decrease the probability of movement along the route from catchment input to presence in the lake; with subsequent potential for uptake by primary producers to produce a biological *impact.* Models that attempt to estimate *State* range from the very simple, requiring crude estimates of catchment attributes or human densities (Cole, *et al.*, 1993) to highly complex, process and distributed, models.

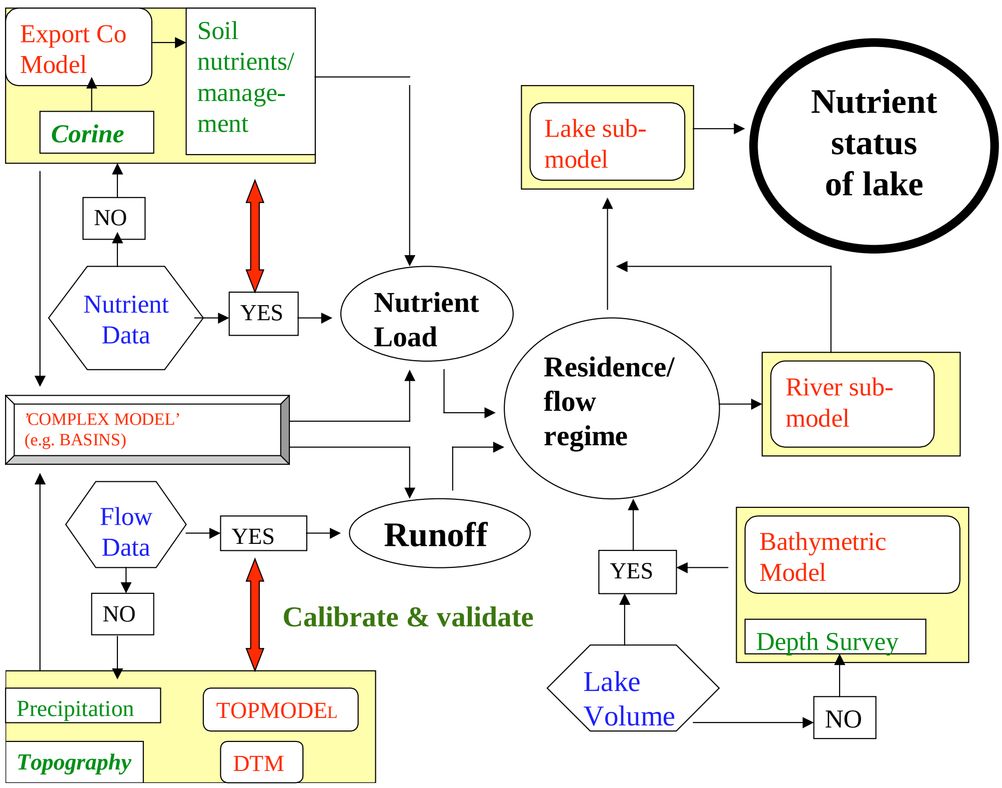


Figure 3.7. A modelling framework, with examples of potentially useful modelling approaches for the assessment on Pressure-State, in relation to nutrients in surface waters.

Catchments are the basic units for modelling and managing water quantity and quality in surface waters. Given a particular location on a river, a catchment is defined as the area which contributes surface runoff to that point. It may be regarded as the set of all points which can influence the quantity and quality of surface runoff water passing that point. While this definition of catchment does not take account of groundwater flow, clearly groundwater needs to be included as an essential feature in the conceptual models of catchment and processes. The WFD places a very strong emphasis on managing the quality of waters and this is, of necessity, inextricably linked with the quantity and temporal distribution of water. For instance, high flows, which cause flooding, are linked with soil erosion and with the detachment and transport of a large part of the distributed-source contaminants in rivers. On the other hand, low flows, associated with droughts, may cause the most ecological harm in a river because of the low dilutions and consequential extreme stress on aquatic and riparian life. Thus, both floods and low flows are as important as average and total quantities.

In general, landscapes are heterogeneous "patch-works" in which spatial pattern and processes interact (Turner, 1989) to produce domains in which either retention of transport of matter dominates (Hagg & Kaupenjohann, 2001). Material within each domain is subject to biogeochemical processes and movement between domains driven by hydrology. The hydrological routing has variable retention and lag-times between inputs and outputs. Catchment models are distinguished by a) the precision of the spatial units used in analysis as being lumped or distributed and b) the precision of the events modelled over time as being a single or continuous event (Maidment, 1993). An example of a catchment model that implements a single event distributed parameter is the Agricultural Non-Point Source (AGNPS) pollution model (Young *et al*., 1989). An example of a catchment model that implements a continuous time step lumped model is the Soil Water Assessment Tool (SWAT) (Arnold *et al*., 1993). Both models were developed in North America and have been significantly tested (Pullar & Springer, 2000).

In general models need to address:

- if and how spatial variability is taken into account. Models can be "lumped" if spatial variability is not taken into account, "distributed" if it is and "semi-distributed" for a partial treatment; and
- how various physical processes are modelled. Models can be "black-box" if no attempt is made to explicitly model the internal physical processes, "conceptual" if simpler analogies are used and "physically-based/deterministic" if the model equations are based on physical laws and relationships. Empirical equations relating important variables are often categorised as "black-box" type.

The conceptual framework of Figure 3.7. identifies potential use of mathematical models. Monitoring, represented by hexagons, calibrates and, on independent data sets, validates the model. Various potential, and alternative, modelling processes are usually possible at each step.

Remote sensing tools will be necessary for characterisation of the River Basin Districts required under Article 5 of the WFD. Landuse across Europe is provided by the EU CORINE (Co-ordination of Information on the Environment) programme. This data is digitally available and provides a foundation for landuse description. Higher resolution remote sensing can be achieved by spectral imaging geared to particular impacts, such as increased chlorophyll concentrations in lake surface waters. Development of remote sensing spectral imaging for this was provided by a recent Irish EPA project (O'Mongain *et al.*, 1999). Representation of catchment landscape by GIS is discussed in Chapter 2.

Issues of Complexity

The following section of the report refers to and reviews models of decreasing complexity from highly detailed process-type models that account for spatial and temporal patterns to simple "empirical black-box" models that, through a series of equations that describe net nutrient movement, are calibrated without detailed knowledge of transport kinetics. All models, however, require initial conceptualisation in order to provide a logical sequence of connections between model compartments. It is also apparent that the distinction between “complex” to “simple” can be a misnomer as the development of “black-box” models evolves towards greater complexity and that of “process” models to greater simplicity.

The principles of solute or particle transport described below are applicable across a range of individual elements. In Ireland the main attention on substance transport within catchments relates to phosphorus as the element that is considered to have the major impact on surface waters and much model development has focussed specifically on this pollutant. While attention on the other main nutrient enriching element, nitrogen, has concentrated on rivers in the south-east of the country, where concentrations tend to be higher than elsewhere, current developments in relation to compliance with the nitrates Directive (91/676/EEC) has extended the geographical focus. Clearly, however, all pollutants that move through catchments relating Pressure to State are amenable to modelling. Indeed transport of many substances, including phosphorus, hitch a ride on particles with release as bioavailable forms related to local temperature, redox and diffusion kinetics. The following addresses, therefore, modelling issues and examples that relate to general hydrological movement, with its solutes and particles, as well as specific reference to individual substances where these warrant separate consideration.

3.3.2. Land and water process catchment models

Distributed catchment models

A distributed catchment model is one in which the spatial distribution of the important catchment characteristics is taken into account. A major attraction of a fully distributed process modelling approach is that it develops an understanding of hydrological processes from the bottom up, through incorporation of the important principles at play. The development of these models was, in-part, spawned by the hope that, once the process algorithms were established, they could then be applied to predict the effects of changes in the catchment without the need for extensive calibration and to predict hydrological run-off at ungauged sites (Beven, 1992). That aspiration has not yet been achieved, as the importance of scale effects and the need for critical observations to reduce model uncertainty are increasingly recognised (Jensen & Mantoglou, 1992).

Distributed models generally require information on topography, channel network, spatial distribution of soil types/properties and of land use/cover and management practices in order to calculate an output. Distributed catchment models can be particularly useful when estimates of sediment load or chemical constituent of the water, such as phosphorus or bacteria, which is mobilised from the soil surface by overland flow, are required. This is because these emissions are not evenly spread across the catchment and most loadings can occur over short periods of time, principally during heavy rainstorms. These models do not, in contrast to lumped models, assume a homogenous flow response to precipitation. This means that models are required which simulate relevant processes at spatial and temporal scales less than that provided by a lumped catchment model. Many distributed models are already linked to GIS systems (and some to a number of different GIS systems). They can be classified into event based or continuous simulation models. The former calculate the total output of the quantities required over a storm event while the latter can produce a time series of concentrations showing the variations before during and after the storm. Implementation of the WFD requires the catchment to be viewed as the integral unit for water management and will, through assessment of risk and *Programmes of Measures*, need to link landuse with water quality. Distributed catchment models permit the detail that might be required to target *operational* and to effect *investigative* monitoring and has been aided by the development of digital spatial data sets for topography (digital elevation models) and hydrologically relevant geographic data such as soils descriptors. Distributed modelling also allows investigation of the sensitivities of model outputs to the individual inputs and can address such questions as effects of (i) data scale, (ii) data accuracy and (iii) correlations among data.

Outputs of distributed catchment process hydrological models are channel flow regimes with, in many cases, water quality estimates. The SHE (Système Hydrologique Européan, Abbott, Bathurst, Cunge, O'Connell, and Rasmussen., 1986) and related models are probably the most widely known example of a distributed model (Beven, 2001). As with any such example, the spatially gridded structure leads to a high demand for data input and parameterisation and, equally, provides for an ongoing process of development to improve incorporation of key hydrological processes and deal with higher spatial resolutions (Bathurst & O'Connel, 1992). In-stream models are considered further in section 3.3.4.

Process-based semi-distributed hydrological models

This class of model are simpler in structure to the fully distributed models.. A key concept is that the response of many grid cells must be similar, and that if their modelling could be done in an integrated way, then this should offer computational and parametric efficiencies. The HBV model (Bergström & Forsman, 1973) is probably the most successful of the semi-distributed models and has been improved and extended continuously since its first used in the early 1970s. It has been used to address water quality issues, e.g. Arheimer, and Brandt, (1998). TOPMODEL (Beven & Kirkby, 1979) is another example, and utilises an index of hydrological similarity (generated from physical data) to guide the process. It has been developed and applied in many environments and is well documented (Beven *et al*., 2001). Its data requirements are much more modest than those of a fully-distributed model. However, TOPMODEL's application does not extend to catchments with important groundwater contributions. Considerable development has been directed at assessing predictive uncertainty, e.g. through the Generalised Likelihood Uncertainty Estimation (GLUE) methodology (Beven and Binley, 1992).

Issues of Scale in hydrological modelling

Issues of scale are anthropocentric. Molecules of sea water dance without distinction to tidal waves, tsunamis, gyres and ripples. Individual molecules of water move through the ground whether in karst tunnels, fractures in rock, macropores or spaces between particles of sand or clay. Scale problems arise only from our efforts to understand, model and predict hydrology. This has necessitated classification and definition of individual processes and, albeit useful but nevertheless often artificial, distinctions between them. This has been extremely useful when examining small and well defined facets of water science. However, scaling problems have arisen with the increasing tendency to (i) expand the scope of phenomena included within such models and (ii) use a wider and more diverse range of sources of information, particularly that obtained as scales different from those at which it is used. This identifies two separate problems: downscaling large scale areal measurements and upscaling small scale measurements to larger scale grids; and upscaling measured data to get "effective parameters" at model computational grid scale.

The modelling process itself produces scale dependence: (i) models are simplifications of reality and often require empirical parameterisations which are sensitive to scale; (ii) the processes being modelled are often nonlinear so that results for one scale cannot easily be obtained from simple combinations of individual results obtained at smaller scales; and (iii) the pressing need is often to model simply the range and character of the complete system response with reasonable accuracy and not to produce a detailed and accurate representation of all its individual components.

Thus, scale problems have arisen as a consequence of the artificial distinctions and limited-scope conceptualisations in water science. For example in another discipline, physicists search for a unified theory of force which reconciles observed (and historically separately named and modelled) behaviour at different scales, e.g. the gravitational, electromagnetic, weak nuclear and strong nuclear forces. Beven (1995) believes such a unified theory in hydrology is not possible; although the quest itself has produced many interesting and useful discoveries and a unified theory is not yet abandoned (for general discussion see Sivapalan *et al*. (1987), Troch *et al.* (1995), Avissar (1995)).

There is a very large use of space and time scales in hydrological models; from consideration of small plots of land a few square meters, to those at tens of thousands of squares kilometers. The purpose of the model, the processes being considered, the type of data available and the hydrological and meteorological regime determine the scale of the analysis. For instance, lumped models may give satisfactory results for some quite large catchments and detailed distributed models may be required for some quite small catchments. Numerous studies of the sensitivity of the model outputs to scale have been undertaken. For instance, scale of the DTM used for topography affects the values of the parameters in TOPMODEL (Franchini *et al.* 1996). However, Saulnier *et al.* (1997) suggest modified extraction procedures to reduce the sensitivity to scale. Time scales tend to depend on the size and response time of the catchment and on the purpose of model use. Typical lumped conceptual models tend to model in time steps from 1 hour up to 1 day. Others are capable of modeling with any time-step. A wide range of different approaches have been used in tackling the scale problem. One problem affecting catchment process modelling is that while this approach attempts to represent surface and sub-surface processes in a physically meaningful way, field measurement of these processes is virtually impossible at the scale, of grid square side length between 50m and 1km, commonly used in the models. Modelling at the catchment scale provides significant challenges, as intrinsic variability of parameters potentially multiply, as well as being non-linear. Addiscott & Mirza (1998) considered that there is no fully satisfactory way of validating a model used at a catchment or regional scale, and that in practice model validation needs to be for much smaller areas, with subsequent test of model efficacy at the larger scales. It is for reasons such as these that necessitate skilled and well-considered application and interpretation of modelling procedures.

Hydrological Response Units (HRU)

An hydrological response unit (HRU) is an area considered homogeneous for modelling purposes. Generally areas with similar land use and physical characteristics are grouped into HRUs. Areas within a particular unit are assumed to exhibit similar relationships between model inputs and output, e.g. rainfall and runoff, and can be modelled with the same set of parameters. A catchment is then considered to be a collection of hydrological response units that differ, in this example, in the relationship between rainfall and runoff. This is a semi-distributed approach and is easily implemented either within or in conjunction with a GIS containing the required land-use, topographical, geological and soils data (e.g. Flügel, 1995). Internal variations within each HRU, or interaction among different HRUs, are not considered in such models.

This general type of approach has been used for quite some time (e.g. Comer & Holtan, 1973) and is seen as a relatively simple way to deal with subgrid-scale variability. For example, within a grid square of a General Circulation Model (GCM), land surface may be categorised into a number of types, with each modelled separately and a weighted average of the results combined to produce the overall results for the grid square (Koster & Suarez, 1992; Pitman, 1995).

The U.S. Geological Survey's Precipitation-Runoff Modeling System (PRMS), a physically-based, distributed-parameter watershed model, simulates runoff for a basin by partitioning areas with homogeneous hydrologic response to precipitation or snowmelt (Laenen, & Risley, 1995; Cary, 1984). Thomsen (1980) used HRUs in a model for a catchment dominated by snow. The addition of radiation information to a snow-melt model allowed Brubaker *et al.* (1996) to include aspect as a factor in subdividing the basin into hydrological response units.

Other authors have called homogeneous units "grouped response units" but have applied the same principles to model e.g. runoff in wetlands from units determined from remotely sensed data (Pietroniro *et al*., 1996), sediment yield from units defined on the basis of topography and soil characteristics (Mashriqui & Cruise, 1997) and for general runoff (Kouwen *et al.*, 1993; Cary, 1984; Shanholtz *et al*., 1981).

Remotely sensed information can e.g. determine the spatial distribution of important factors such as topology, land use, and monitoring flooded areas. Kite & Kouwen (1992) have shown that a semi-distributed model using sub-basins derived from Landsat images performed better than a lumped model. GIS allow spatially distributed information such as topography, soil type, rainfall distributions or soil moisture distributions to be easily included in models. For example, Kouwen *et al.* (1993) applied a Grouped Response Unit (GRU) using satellite land use data and a computational element of either a sub-basin or an area of uniform meteorological forcing, for modelling. In HYDROTEL, Fortin & Bernier (1991) suggest combining SPOT produced DEMs with land use and soils mapping data (perhaps also remotely sensed) to define Homogeneous Hydrologic Units (HHU). Ott *et al*., (1991), and Schultz, (1993) have defined Hydrologically Similar Units (HSU) using DEMs, soils maps and satellite derived land use information to study the impact of land use change in the Mosel River Basin.

Some authors (Duncker *et al*., 1995) have used sub-catchments as HRUs, while others have used finite flow routing elements, for instance the Finite Element Storm Hydrographic Model (FESHM), to represent catchment unit response area, characterized by a single set of hydrologic (HRU) properties (Heatwole *et al.*, 1982). Even more generally, HRUs have been used as a basis for an object oriented approach to catchment model implementation (Whittaker *et al*., 1991). This was a response to the increasing complexity and scope of hydrological models required for environmental applications. It utilises the concepts of objects which can have attributes and behaviour (i.e. a catchment or sub-catchment can be an object, rain can be generated by an objectly). Objects can communicate between each other by sending messages and have properties of inheritance and modularity. In an object-oriented approach, much of the programming complexity associated with these properties is handled by the programming language, reducing the programming burden and increasing the flexibility both in extending and upgrading the resulting model. The HEC-HMS (US Army Corps of Engineers, Hydrologic Modelling System) is perhaps the best known example of this approach.

Representative Elementary Area (REA)

Wood *et al.* (1988) proposed The Representative Elementary Area (REA) as the minimum topographical scale with which it was reasonable to represent a catchment's operation with a simple lumped model. For runoff generation on a test catchment using the TOPMODEL distributed model, the REA appeared to be approximately 1km, and strongly influenced by topography. Other work has suggested that REAs varied between the order of 5 - 10 km^2 for one catchment and 1 - 2 km^2 for another. Blöschl *et al.* (1995), using measured river flows, concluded that length or area scale depended on duration of rainfall, with large-scale variation controlled by precipitation and small scale variability by soil properties and topography. Precipitation-runoff models are capable of simulating with good accuracy when there is sufficient calibration and raingauge coverage (Letcher *et al*., 2002).

Regional precipitation-run-off Modelling

Current work in Ireland (Holden *et al*., *submitted*) has developed a conceptual model of catchment run-off risk that is defined at a regional scale. The conceptual model assumes that runoff/pollution is an open system that interacts with its environment. From this point-of-view, rainfall climate is an external stimulus, providing the transporting agent – water, that interacts with the system and that the soil environment can be considered as a simple two state situation (Daly *et al*., 2002; Brereton, 1989) with poorly drained/high water table soils, and the others. This idea is supported by the contention that the effective depth of interaction is not necessarily influenced by soil type during runoff events (Ahuja *et al*., 1981). It is assumed that runoff is most likely to occur on soils that are in excess of field capacity and, therefore, most likely on poorly drained and/or high water table soils. The conceptual model assumes that is should be possible to predict when significant risk of runoff might occur for other soils based on rainfall patterns. To date the idea has been applied using a climate time-frame (30+ years) and a regional spatial scale to produce winter runoff risk maps (Figure 3.8). It is difficult to independently test the methodology. However, ongoing research is examining the potential application of the concepts to forecasting for smaller areas such as fields by using land unit classification (Conacher and Dalrymple, 1977) and numerical weather prediction models. This approach will provide a test of the conceptual framework of the idea.

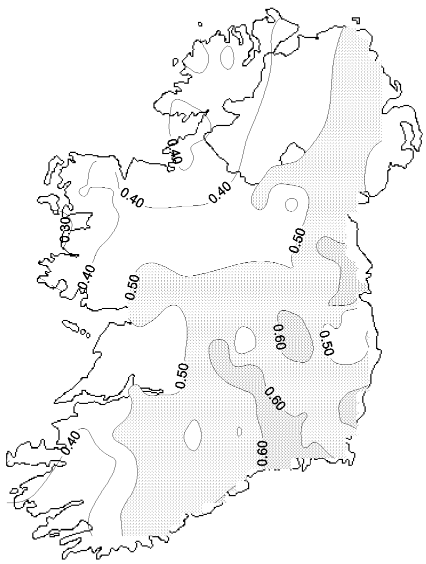


Figure 3.8. Map of runoff risk defined using 40 years of rainfall records for 151 rain gauges examined using an 8 day rainfall threshold pattern (2.5-2.0-1.5-1.0-0.5-1.0-1.0 mm). After Holden *et al.* (in press).

A new design of rainfall-runoff models is represented by Génie Rural models (GR) that favour a simplistic structure to increase robustness and reliability of the model. The input into GR models is limited to fundamental and easily available parameters such as rainfall, streamflow and evapotranspiration and the models are based on a global analysis of the catchment hydrological behaviour. GR models stand in contrast to physical based models used for rainfall-runoff estimates that are of great complexity. The high number of parameters needed for these latter models causes calibration problems and often uncertainty of source data. The French group Cemagref developed and tested GR models extensively and recommend their use within the WFD for reservoir management, detection of human impact and flow forecasting (Andréassian *et al.,* 2001).

3.3.3. Transport from land to water: empirical "black-box" models.

Empirical models do not reveal hydrological or other specific features of the catchment, but can estimate net transport and pollutant loads quite effectively, and be responsive to management and climatic drivers. While the use of these models can have a great advantage of conceptual and mathematical simplicity (Johnes *et al*., 1996; McGuckin *et al*., 1999; Jordan *et al*., 2000), they are, nevertheless, increasingly in their complexity in order to account sufficiently for spatial and temporal complexity of material transport (Behrendt *et al.,* 2002; Heathwaithe *et al.*, 2003).

Nutrient export coefficient models

The complex dynamics of catchments make it difficult to estimate nutrient budgets (Lowrance *et al.,* 1985) or, indeed, transport of any material. Maximum phosphorus loads and concentrations often occur following high rainfall (e.g. Lennox *et al.*, 1997) and, unless monitoring regimes are at high temporal resolution, nutrient pulses associated with short flood events may be undetected. Sampling at high temporal resolution provides high quality data, but is generally not possible owing to logistical and cost constraints. An alternative approach to the long-term and continuous measurement of nutrient and hydraulic transport is to estimate nutrient loads through a knowledge of catchment geology, topography and landuse. Such empirical modelling has commonly employed the use of export coefficients (e.g. Uttormark *et al.*, 1974; Beaulac & Reckhow, 1982; Clesceri *et al.*, 1986; Johnes,, 1996) or multiple regression analysis (e.g. Håkanson & Peters, 1995; Daly *et al.*, 2002; Johnson, *et al.*, 1997). These approaches generally ignore the processes of loss and supply, including the complexities of soil-phosphorus interactions, although Daly *et al.*, (2002) included knowledge gained from experimental phosphorus desorption studies in the development of regression models that predicted molybdate reactive phosphorus (MRP) in rivers from land use categories that reflected high or low grassland productivity and soil-P status. Separate regressions were used for well- and poorly-drained soils.

A nutrient export coefficient modelling approach was advocated by Johnes *et al.* (1996) to predict nutrient loads to surface waters and was applied across a range of UK catchments varying in landuse and topography. It is an attractive management tool that does not involve either long-term and intensive chemical and hydraulic measurements or the understanding of soil-phosphorus kinetics. If common export coefficients can be applied across a range of catchments to estimate in-lake concentrations of phosphorus with high reliability, the need for widespread sampling and chemical analysis in lake monitoring programmes could be radically reduced. In a test of this model (Irvine *et al.*, 2000) found that while mean TP in Irish lakes were, by and large, ranked successfully, the predictive power for the quantitative estimation of mean TP concentrations was modest with $r^2 < 0.4$ ($n = 29$). The model also tended to overestimate measured concentrations. Similar results were found for the Johnes model (Johnes, *et al.*, 1996); by Valiela *et al.* (2002). Nevertheless, the development of simple empirical relationships between key features in the catchment and lake nutrient status merit further development as the potential to reduce the need for intensive data collection is highly cost-effective. In addition, even if model predictions are not quantitatively robust, application of export coefficients to rank risk of surface, and groundwater, degradation provides a powerful management tool.

The Johnes *et al*. (1996) modelling approach applies export coefficients determined for a variety of different land use and livestock stocking regimes. A simpler approach using only land-use categories identified by the Co-Ordination of INformation on the Environment (CORINE) satellite remote sensing was applied by Jordan *et al.* (2000), using export coefficients determined by McGuckin *et al.* (1999) to predict phosphorus loads from over 50 river catchments in N. Ireland. In a test on independent data, the export coefficient models predicted well annual TP loads to the River Robe catchment in Co Mayo, but not those of nutrient loads to Lough Carra (Irvine *et al*., 2003). The discrepancy between the modelled P loads to the two lakes, relative to those measured, is likely mainly because of differences in hydrological connectivity with surface waters, with perhaps additional influence of variations in soil phosphorus concentrations between the two catchments. Error that may arise from infrequent monitoring are probably insufficient to explain the disproportional differences in estimated total P loads to the lakes.

The Johnes (1996) model also hindcast loads modelled back to the 1930s as a mechanism to gauge a state-change in nutrient loadings; a technique that could also be employed to set modern targets of nutrient loads. Hindcast loads can help estimate chemical reference state, which through appropriate calibrations can further model biotic conditions. Aerial photographs to estimate changing pattern of landuse, were employed by Valiela & Bowen (2001) to help estimate historical N loads to Waquoit Bay, Massachusetts.

A number of other export modelling approaches are described in the literature. Some of these, MONERIS (Behrendt *et al*., 2002) *Realita* (Kirk McClure Morton, 2001) and N-LES (Simmelsgaard *et al.*, 2000) are currently been compared, along with more process orientated models (TRK, SWAT, ANIMO), as part of an EU project EUROHARP designed to quantify nutrient losses from diffuse sources across 17 study catchments incorporating a range of European climate, soils, topography, hydrology and land use (Table 1.2). MONERIS**,** designed to estimate catchment N-loads has been tested across a number of European catchments, including that of Lough Mask in Ireland (Venohr *et al*., 2003). The MONERIS model appears more successful for larger compared with smaller catchments and also needs high level of detail of data input. In contrast, the *Realita* model (Kirk, McClure and Morton, 2001) requires very limited data input: organic fertiliser loads, land use and risk of run-off to surface waters; soil phosphorus measurements; and mineral fertiliser loads. Output is a risk score based on ranking of input characters. The scope of the model is limited and has not yet been critically evaluated in the literature. Its main value appears as a qualitative guide to management decisions. Nutrient exports coefficients linked to models of sediment loss for P and denitrification of N is applied in the Australian ANNEX model (Young *et al*., 2001). This is a national model utilising nutrient and flow data, collected at fixed gauging stations. The model demonstrates the implementation of a national approach to the estimation and modelling of nutrients across river networks. See also description (below) of the SPARROW model (Smith *et al.*, 1997).

Recent work (Heathwaite *et al*., 2003) has developed the empirical modelling of diffuse P export with a conceptual framework of three layers- storage, mobilisation and hydrological connectivity-for which the data input of each can be expanded and refined as knowledge and information become available. The model is a synthesis of three existing modelling approaches developed in the U.K. by, respectively: Johnes (1996); Johnes, *et al.* (1998); Harrod & Fraser (1999) Harrod & Fraser, (unpublished MAFF report) and Withers (unpublished MAFF report) and is designed to support management options (Heathwaite, 2003). Key attributes of P Indicator tools claimed by Heathwaite *et al.* (2003) are:

- An ability to operate across a range of scales and applications using the same framework, but with scope to modify the coefficients sets used at different scales;
- Clear assumptions built into all layers; and
- Calculations and parameters are as far as possible designed to be derived or tested against field measurements.

Within Layer 1 the model uses spatial data input of livestock, crop and topsoil mineral density to estimate, from landuse/animal specific coefficients, loading of phosphorus within 1 km^2 grids within a catchment. This provides an index of potential P loss, that is modified by layer 2, P transfer indicators. The main drivers within Layer 2 are soil characteristics, climate and slope. The Hydrology Of Soil Types (HOST) classification (Boorman *et al.*, 1995) is used to apportion P transfer to surface and subsurface flow pathways, although currently this does not utilise the full potential of the HOST system as it only distinguishes between broad categories of grassland and arable landuse. Coefficients are applied to Olsen P concentrations, manure and fertiliser input and particulate soil loss to estimate P transport from the edge of a notional within field plot. The approach separates pathways of dissolved reactive P and particulate P. The realisation of P export to surface waters is dependent on Layer 3, P delivery indicators. The key control of this hydrological link is through coefficients that predict: the degree of sediment retention within field and ditches; the extent of artificial drainage; and the distribution of routes of high connectivity. Many of the transport links and associated coefficients cannot currently be quantified because of limited or contradictory data. While the P tools model has been tested on two contrasting U.K. catchments, its strength appears to lie in having a well defined conceptual basis, which lends itself to incorporation of empirical data as this becomes available.

The modular approach of P Tools helps identify most critical internal mechanisms through which changes in model inputs affect predicted P loss and concentration. However, each calculation stage in each layer of the model has uncertainty arising from spatial input data and assigned coefficients. For many of these stages there is very limited available data. For example, spatial data, often based on census data at resolutions of parish boundaries (in Ireland this restriction would apply to DED resolution) restricts the model, which is designed to operate at both finer grid (1 km^2) and larger (catchment) scales. Other areas that the model requires development would be in defining the relationship between P mobility and weather, particularly storm flows and antecedent moisture conditions (Jennings *et al.*, 2003). Nevertheless, the model has potential for current application in that it can help identify areas and activities of high risk of diffuse loss of P to surface waters. As such it may have a useful, and cost effective, role in the characterisations of catchments and estimation of risk to surface waters required under Article 5 of the WFD, which is also an early requirement (by end 2004) of the implementation schedule. Scenario analysis using a model such as P Indicators Tool has, in addition, application for implementation of *Programmes of Measures* under Article 11 of the WFD. These requirements suggests that modelling approaches such as that provided by P Indicator Tools, or some of the simpler, but related, approaches are indeed a necessity to guide implementation of the WFD. P Indicators Tools was developed for use within an Arc/Info GIS framework, using raster or grid-based data. The P Indicators Tool model has similarities to other models using simple nutrient indexing approaches to help management of diffuse P loads (Gburek *et al.*, 2000), models such as GWLF (Haith *et al.*, 1992) that parameterise land-use spatial patterns, or simple empirical spreadsheet techniques (Walker *et al.*, 1989).

Export flux

An adaptation of the export coefficient approach that employs GIS to identify land-use categories and distance of pixels to a path of surface overland flow is suggested by Soranno *et al.* (1996). The technique was developed to model particulate P movement, with the underlying conceptual model that P delivery to surface waters is by attachment to particles (Novotny & Chesters, 1989). This view is adopted by a number of models designed to estimate P load from land to water. While this has been challenged, especially in grasslands (see Jennings *et al.*, 2003 for review), it is probably reasonable for arable-dominated catchments. In these settings, sediment delivery ratios decrease with catchment area (Walling, 1983). Various processes between source and receiving waters may attenuate P transformation and transport in both arable and grassland catchments (Jennings *et al.*, 2003). The model of Soranno *et al.* (1996) incorporates an attenuation coefficient that accounts for loss of P between pixels, and estimates net delivery to surface water based on distance from source to stream. These concepts are also employed in P-Tools indicators (Heathwaite *et al.*, 2003). Further, Soranno *et al*. (1996) only included “contributing areas” of the catchment; which may be equal or less than the whole catchment. Overland flow in grassland catchments is a response to hydrological saturation, and occurs, in what have been termed as *variable source areas* (Sharpley & Rekolainen, 1997).

Regression Models

Although multiple regression models may appear intuitively more complex than an export coefficient approach, the computational requirements are straightforward and data requirements can be less demanding than the more elaborate export-coefficient type models such as P-Indicators Tools and MONERIS. Simple regression models can be used to link status features of the catchment with mean concentration of a given variable in surface and groundwaters. Techniques are described in Håkanson & Peters (1975). Daly *et al.* (2002) used a multiple regression approach to model mean loads of phosphorus to Irish rivers based on soil properties and land management. Models relating static catchment descriptors such as extent of land cover by a vegetation type or soil properties are constructed across catchments and present model outputs of *average* conditions. Håkanson & Peters (1995) demonstrated that regression analysis based on simple to obtain “map” variables explained most (ca 60%) of the variation in annual measures of in-lake total phosphorus. However, in a further critique, Håkanson (1999) demonstrated that regressions with $r^2 < 0.75$ could be considered effectively useless for lake management. An alternative approach is the use of regression to model nutrient loads with a single catchment (Portielje & Rijsdijk, 2003) using a series of relationships calculated from measured variables. This technique requires more intensive sampling and more computational sophistication.

Regional spatial network model-the -SPARROW model

Within the requirements of the WFD, characterisation of the catchment, risk assessment and monitoring networks are clearly linked. Targeted *operational* monitoring is required for water bodies that are *at risk* of failing to reach environmental objectives. *Operational* monitoring is a tier of intensity greater than *surveillance* monitoring, which can be viewed as a routine validation of the maintenance of *good* or *high* status. A regional modelling approach for the estimation of water quality based on land use attributes and the existing, or future, monitoring network of the Irish EPA provides a necessary screening tool. The SPARROW model developed by the US Geological survey (Smith *et al.*, 1997) uses spatially referenced regressions of pollutant transport to estimate compliance to water quality targets. The method predicts water quality metrics as functions of river channel and catchment descriptors, including measurements and parameters that describe point and diffuse pollutant loads, and includes coefficients for transport efficiency.

Regional modelling can reduce commonly encountered problems of network sparseness, bias and catchment heterogeneity. Estimates of water quality are often based on frequency-related interpretations of monitoring data (e.g. DELG, 1998), which can be undermined when spatial or temporal biases are large. The SPARROW model employs a somewhat similar conceptual model as P-Tools by recognising the importance of spatial heterogeneity and weighting of zones of influence (Soranno *et al.*, 1996; Cressie & Majure, 1997) and models transport in streams as a function of referenced land-surface and stream channel characteristics. Statistical “bootstrapping” techniques provides robust error measurements of modelled pollutant loads. Application of this, or a similar model, appears highly appropriate and feasible in Ireland given recent developments of a national Digital Terrain Model, and availability of CORINE remote sensing information.

Recommendations: Simple export coefficient methods such as relating average P-loss from land-use categories identified in CORINE can be efficient risk assessment screening tools to be used in characterisation of catchments. Use of more complex empirical models such as P-Tools and SPARROW can provide further detail necessary for identifying critical source areas and application in operational and investigative monitoring in catchments where water bodies fail or are at risk of failing to reach their environmental objectives.

3.3.4. Linking catchment with in-stream hydrological and water quality models

Predicting water quality is a more uncertain endeavour than predicting hydrological regime. To model water quality well using physically-based models requires good conceptual models of the hydrological cycle. In particular, it is important that models determine correctly the proportion of effective rainfall which is split between surface runoff and infiltration. Any uncertainties or errors in the hydrological fluxes will carry through to the modelling of water quality. The model must then simulate the production, transport, transformation and deposition of contaminants. Approaches tend to be specific to the contaminant in question, but may involve a dissolved or particulate form of the contaminant or both. For instance, sediment is modelled as a particulate contaminant, and is transported by overland and channel flow. Nitrate is a dissolved contaminant and can infiltrate to groundwater as well as contaminating surface runoff. However, phosphorus can occur in both forms and can change from one to the other as it is transported. The difficulties of effect of scale on modelling catchment nutrient movements compound those of hydrology.

Reviews of modelling systems have been prepared by the Natural Resource Conservation Service of the U.S Department of Agriculture (Natural Resource Conservation Service, 2000) and the Water Environment Research Foundation (2000). Chapra (1997) provides a thorough discussion of surface water-quality modelling and Singh (1995) provides an extensive description of 26 commonly used hydrology models, applicable to civil engineering and catchment management. Some of the models described in Singh (1995), such as HSPF, SHE, TOPMODEL, MIKE 11 are also referred to in different sections of this report as those that have been used or seem applicable to use in Ireland. Others, such as AGNPS, CREAMS, EPIC, GLEAMS, SWRRB, are also included in a review of in-stream models done as part of the Irish River Basin Three Rivers Project (The Three Rivers Project, 1999). Models described in that report address water movements, sediment transport and water quality. There is, as would be expected, overlap in modelling approaches to rivers/streams and estuaries. CREAMS (Knisel, 1980) and GLEAMS (Leonard *et al.*, 1987), used widely for agricultural management in the U.S., focus on overland flow pathways to water courses. In the Netherlands, the ANIMO model (Groenendijk & Kroes, 1999) is used to predict nutrient load to surface waters and nitrate concentration in upper groundwater zone. ANIMO is an integrated hydrological/leaching model which has been applied at field to regional scales (Groenendijk, 2002).

Movement of material thorough catchments is dependent on rates and pathways of water flow. In channels hydrodynamics of advection-dispersion and material transport underpins most simulation modelling (Metelka & Krejcik, 2002). Open channel hydrodynamics can be represented in 1, 2 or 3-dimensions. 1-D models are often used for analysis of a system over periods of years, and are frequently used to forecast overflow in sewerage systems. 2-D models are employed where detail along the horizontal axis is required and where variation along the vertical axis has no significant influence, or is not required. If such is not the case a 3-D model is appropriate (van Waveren *et al.*, 2000). Hydrodynamic models are generally based on the conservation of mass and momentum.

Given the requirements for hydrological data and the frequent lack of measurements for points of interest, it is no surprise that hydrological modelling, in which simulation and prediction of river flows (often termed streamflow) is the object, has a long and rich history (Singh, 1995). Input data include - at a minimum - precipitation data at a time resolution appropriate to the application, but may also include evaporative and other more detailed meteorological variables, and may or may not include data relating to the catchment. Model applications are numerous, including flood forecasting, pollution forecasting, water resources planning, in-stream habitat modelling, and various assessments of the impacts of climatic or land use changes. Stream-flow models require gauging station calibrations.

For the WFD, one of the most important applications of hydrological modelling may be the generation of stream-flow time series as a component of assessing the ecological status of water bodies which have been subject to anthropogenic alteration, such as rivers downstream of a water abstraction or a hydro-electric reservoir/power station.

Black-Box (empirical) hydrological models

As described for catchment models above, this class of model makes general functional (e.g. regression models for the linear case) relationships between input and output. The unit hydrograph model is a classic example and efficient ways of implementing it have been published (Bruen & Dooge, 1992). Classical time-series models, such as ARMA models (Box & Jenkins, 1970; Weeks & Boughton, 1987), are another example. A variety of different terms have been applied to this type of modelling, including "data-based mechanistic approach" (Young and Beven, 1994). In the latter, the data is allowed to determine the model form as much as possible (Beven, 2001), although mathematically, the models are simple numerically, the parameter estimation is ill-conditioned (small errors in the data can lead to large estimation errors) and requires special methods best executed by a experienced hydrologist with an understanding of modelling.

A development of the simple "black-box" in-stream models are those that use a highly simplified description of a catchment, generally using a simple analogy. Typical analogies are a simple store (bucket, representing the continuity or conservation law) and a linear reservoir, which combines a linear dynamic outflow relationship with the conservation law. Typically, models will involve some sort of filter which separates precipitation into effective (i.e. contributing to quick-flow) and ineffective elements. Conceptualisations of two pathways between input and output are then used, representing quick-flow and slow-flow processes, and these may contribute to streamflow either in parallel or in series. However, there is no opportunity for the link between these conceptual pathways and physical processes to be examined, let alone verified. The IHACRES model (Jakeman *et al.*, 1990; Littlewood & Jakeman (1994) is a well-used example of a data-based hydrological model, used for hydrograph analysis to e.g assess impacts of land-use or climate, change and quality assurance of long, strategically important, hydrometric records.

Integration of hydrological elements.

In any particular situation there may be a need to incorporate a range of hydrological and water chemistry components into a model. Some of the more complicated and larger process distributed and semi-distributed models enable this. In many "black-box" models the output is a net consequence of a range of processes. There is, however, increasing, modular approach to modelling. One example is the SOBEK family of models (***www.sobek.nl***) which provides a package that address river and estuarine flow, morphology and hydrochemistry, and organised as an open modelling system, which also facilitates subsequent links with external modules.

Water quality changes in rivers result from physical transport and biological, chemical and physical conversion processes. River models have traditionally considered changes of substances concentrations along a river length to be consequential on advection + diffusion/dispersion + conversion processes. The best developed models address point source pollutants and have evolved from the early work of Streeter & Phelps (1925) that described the increase and following decrease of the oxygen deficit downstream of point-source input of organic load. The current industrial standard is probably the QUAL2E (Brown & Barnwell, 1987) model that simulates dissolved oxygen and associated water quality variables and incorporates degradation of organic matter, growth and respiration of algae, nitrification, hydrolysis of organic nitrogen and phosphorus, reaeration, sedimentation of algae, organic phosphorus and organic nitrogen, sediment uptake of oxygen, and sediment release of nitrogen and phosphorus. It is a steady-state model that was derived directly from the U.S. regulatory framework for which it is generally well suited. It assumes steady-streamflow and steady-effluent-discharge and was not designed for temporal variations in streamflow or for where major discharges fluctuate over diurnal or shorter time periods (Shanahan *et al*., 1998). Other well used models such as the Danish developed MIKE11 (DHI, 1992) and or German Allgemein verfügbares Gewässergütemodel (ATV, 1996) are better able to simulate transient conditions. MIKE11, in contrast to QUAL2E, also partitions organic matter into dissolved, suspended and sedimented fractions and enables changes in sediment quality to be incorporated in the model. Further comparison of these models is given in Rauch et al. (1998). In general, however, there is currently no generally available and widely accepted water quality river model that deals effectively with large fluctuations in diurnal conditions and situations for which diffuse sources provide a significant input of nutrients. In addition, the expertise needed to run models such as QUALE2 and MIKE11 is high; without which the user may lack the depth of understanding needed to evaluate the applicability of the model to the problem at hand (Shanahan *et al*., 1998). With increasing emphasis on the importance of diffuse nutrient loads to surface waters, and the recent verification of the importance of field nutrient emissions from Irish catchments that lack any point sources (Jorden, unpublished data), there is a need to develop models that can simulate cumulative inputs and losses of nutrients in Irish rivers. However, given the difficulty of developing process models for that purpose, it is unlikely that such models applicable for widespread use in Ireland will be forthcoming in the near future. Furthermore, simpler nutrient models such as SIMCAT (NRA, 1990), used by the UK Environment Agency, that address point sources are generally applicable only if the contribution of point source dominates total nutrient loads. Recent and current upgrading of many SWT plants in will reduce the contribution of many sewage treatment plants to total P load. Modelling may, of course, still have an important role in determining whether investment in P-removal technologies is required in order to meet compliance targets.

Detailed modelling of in-land point-sources is likely only of importance where there is a failure to meet environmental objectives *and* where there is sufficient uncertainty of the casual conditions or mitigations necessary to justify a complex model. The need for modelling in coastal and estuarine situations, subject to a greater range of pollutants, often in higher concentrations with greater potential for impact, and subject to more complex hydrodynamics is likely to be higher.

An example of a recent development to address the limitations of river water quality models described above is the River Water Quality Model no 1 (RWQM1) produced by an International Water Association Task Team, set up to create a technical base for standardised, consistent river water quality models and guidelines for their use. This work was instigated to develop water quality models that are compatible with existing IWA Activated Sludge Models (Henze *et al.,* 1987; Henze *et al*., 1995; Gujer *et al.*, 1999). Shanahan *et al*. (2001) describe a six-step process to guide decisions on model structure applicable to the range of river conditions that fit the River Continuum Concept (Vannote *et al*., 1980). These are summarised as:

Step 1: Definition of the temporal representation (dynamic compared with steady-state) that focuses on transport terms of the model and requires listing of all characteristics time constraints of relevant processes;

Step 2: Selection of spatial dimensions, including if and how the sediment is included in representation of the river;

Step 3: Determine representation of mixing, which depends on step 2 and number of dimensions to be modelled. Whether modelled as dispersion or diffusion, the represenation of mixing varies depending on the hydrometrics of the site;

Step 4: Determine representation of advection which, like step 3, does not depend on the characteristics of the conversion processes and can be, indeed, modelled independently of the water-quality;

Step 5: Selection of the biochemical submodels, and their reaction times. This step is treated in more detail in Reichert *et al* (2001) and Vanrolleghem *et al.* (2001);

Step 6: Determine boundary conditions, which is intrinsically linked to choice of model dimensions;

Shanahan *et al.* (2001) conclude that construction of a river water quality model must be based on the logical develop of the elements in the model. These will vary with local conditions. The framework they outline provides a suitable example that the details of, especially the more complex, models and choice of algorithms vary with the question in hand. The parameters in such "state of the art" models are not universal enough to apply across systems (Reichert & Vanrolleghem, 2001). This is a crucial general point that merits frequent reiteration, and could apply to even the simplest of useful models. Early case studies using the framework of the RWQM1 are discussed in Borchardt & Reichert (2001) and Reichert (2001).

3.3.5. Modelling nitrogen

The models described above relate mainly to phosphorus transport. While the principles that are employed in P-loss models can be applied to a number of elements, sufficiently important distinctions in the mechanisms of nitrogen transport merit special consideration. While a common opinion would be that P is of prime importance for surface water enrichment of inland waters and N of greater importance in coastal and ocean areas, this is only true in a very general sense. The management and understanding of the mobility of both nutrients is important for the implementation of the WFD for the protection of surface and groundwaters from eutrophication. A conceptual model of the N-cycle would generally be considered to involve a greater number of steps than that of the P-cycle. While the movement of P through catchments and waters is basically a process of attenuation and onward, down-slope, mobility, that of N also links with the atmosphere. For this reason also, its management is of major consideration for climate protection as human activities have disrupted the global N-cycle (Vitousek *et al.*, 1997).

In rural landscapes, the N-cycle is disrupted by intensification of agriculture, leading to increases in nutrient, mainly nitrate, loads to surface and groundwaters, emission to atmosphere as nitrous oxide and ammonia compounds and, through atmospheric conversion, acid deposition. Estimated average anthropogenic load of N into the catchments draining to the North Atlantic are 39 kg ha^{-1}, of which about 40% eventually discharges to the sea (Howarth *et al.*, 1996). Losses through the catchment are through harvest, retention, denitrification and volatilisation as ammonia. Leaching to groundwater is also important, and results in vary variable retention times. Additional input is through biological fixation of nitrogen gas.

Point and field scale models of N-movement (e.g. DRAINMOD-N, DRAINMOD/CREAMS) are primarily of research interest for understanding the processes and not applicable to the catchment scale (Hagg & Kaupenjohann, 2001); although such models developed at small spatial scales are often expanded to the catchment scale. While, therefore, probably not directly useful for implementation of the WFD, they are clearly important in developing the models that are (see de Willigen & Neetson (1985); de Willigen, (1991) for comparison of N-simulation models in soils).

Large scale catchment models (e.g AGNPS, ANSWERS, N-LES, NLOAD, SOILN), estimating N loss to surface or groundwaters have applied both a nutrient export coefficient (Johnes, *et al.*, 1996; Valiela *et al.*, 1997) and more process type (e.g. Johansson *et al.*, 1987) approach. The complexities of scale (e.g. Blöschl & Sivapalan, 1995), unpredictability of transport pathways (e.g. Bouma, 1992), importance of extreme events (Petersen *et al.*, 1987), together with the importance of transfers and links with the atmosphere, has led some authors to conclude that an accurate quantitative prediction of N dynamics and nitrate loss from agricultural systems as seemingly impossible (Jury & Flühler, 1992; Richter & Benbi, 1996). This somewhat pessimistic view may reflect too great an expectation of the models. The study by Valiela *et al.* (1997) estimated modelled N loads to an estuary to within 38% of the mean recorded values and led the authors to conclude that their Nitrogen Loading Model is better used to produce "fuzzy" guidelines for overall net loads. In further work (Valiela *et al.*, 2000), this model used stable isotope ^{15}N to partition source loads to an estuary. Models developed for lowland agricultural systems (Addiscott and Whitmore, 1987; Cooper *et al.*, 1993) tend to be dynamic models that provide short-term (i.e. weekly) information.

Models such as AGNPS considers separate land parcels as distinct, but hydrologically connected and has been used widely in the U.S. (e.g. Bhuyan *et al.*, 2003). AGNPS uses a series of sub-models that address hydrology, soil erosion and nutrient pollution (nitrogen, phosphorus and chemical oxygen demand) and can include a GIS Arc-Info interface. It is, however, limited to single event simulation and to catchments not larger than 10 km^2. Recent work to link the nitrogen transport model SOILN (Johansson *et al.*, 1987) and a soil and heat model SOIL (Jansson and Halldin, 1979) into a modelling framework designed for management decision support is described in Johansson *et al.* (2002) and provides an example of an attempt to simplify complex models to facilitate more general use.

A nitrogen model for river systems that take into account instream nitrification and denitrification is QUASAR (Whitehead *et al.*, 1997), which has been applied to large river basins (Whitehead, 1990; Whitehead and Williams, 1984). A recent model by Lunn (1995) addresses the whole catchment in a distributed manner but is driven by the complex hydrological model, SHE (Système Hydrologique Européen; Abbot *et al.*, 1986).

Valiela *et al.* (2002) compared ten process and empirical models for the estimation of N loads from land to shallow estuaries, and found that the more complex models tended to be more responsive and precise, but not necessarily more accurate or predictive. Different models varied quite considerably in the partitioning of land-derived N-sources, which indicates that although overall estimations of net N load may appear verified, there is clearly uncertainty within the model of sectoral contributions. This could have important consequences for management or implementation of *Programmes of Measures* by directing effort and cost inappropriately.

In Ireland, pressure through failure to fully implement the Nitrates Directive (91/676/EEC), proposed designation of Nitrate Vulnerable Zones, general concerns of N loss to surface and groundwaters and loss to atmosphere, coupled with historic concerns of importance of N for agricultural efficiency, has prompted considerable interest in understanding processes of N-flux through catchments. An N-leaching model, NCYCLE (Scholefield *et al*., 1991), is currently under development, with funding from Teagasc, for use in Irish grasslands. NCYCLE is an empirical mass balance model of annual N transformations in grazed and cut grasslands. It assumes that annual N inputs such as fertilizer additions, mineralization and atmosphere deposition are balanced by the removal of N in animal product, losses to the environment through leaching, denitrification and volatilisation and accumulation in organic matter. NCYCLE makes adjustments for sward age, climatic zone, soil texture and drainage status, with mineralization rates increasing with age of sward, temperature, clay content and drainage. Application of the model in comparison with the CENTURY model designed to simulate long-term dynamics of carbon, nitrogen, phosphorus and sulphur, has been reviewed by Bhogal *et al.* (2001). The minimum input requirements include climatic zone, sward age, texture, drainage, history of sward, fertiliser applied and livestock management. The user can adjust N inputs, soil and background management conditions, in order to predict effects on production N off-take, transfer and losses. The model is user-friendly and does not require detailed knowledge of soil layer hydrology, N transformations or computing. Limitation to the model may, however, arise by the inherent complexity of the processes involved in water movement and N cycling, and imprecision of data available as inputs. Model output is a prediction of annual N leached from the soil. Like most mass-balance and catchment models it is insensitive to seasonal patterns. It also does not provide predictions of nitrate concentrations to surface water.

Modelling of N runoff and impact has been progressed by the EU funded INCA model (see *www.rdg.ac.uk/aerc* for further information). The model simulates flow, nitrate-nitrogen and ammonium-nitrogen and tracks both terrestrial and river flow pathways. The model is dynamic and can simulate daily variations in flow and nitrogen following a change in input conditions such as atmospheric deposition/sewage discharges or fertiliser addition. The model can also be used to investigate change in land use. Dilution, natural decay and biochemical transformation processes are included in the model as well as the interactions with plant biomass such as nitrogen uptake by vegetation. Development of the model is described in Whitehead *et al.* (1998a) and test of its use in Whitehead *et al.* (1998b). Development for a 'sister' phosphorus model INCA-P is in progress.

Recommendations:

- Further development of nitrogen leaching models, especially in Irish grasslands is required. Understanding of the processes are important, although often difficult, challenges in order to implement sound management to meet the needs of the WFD and Nitrates Directive (91/676/EEC).
- The INCA model was developed specifically with the Water Framework in mind. Its application to Irish rivers should be investigated.

3.3.6. Current use of nutrient models in The Republic of Ireland

As part of the *EPA/Teagasc* on effect of agriculture on water quality there are a number of modelling activities. These include development of precipitation models decribed above, a comparison of the performance of SWAT, HSPF and SHETRAN for modeling P loss is currently ongoing for the Clarianna catchment in Co Tipperary, the Dripsey in Co. Cork and the Oona water in Co. Armagh. Realising that a large number of models have been developed and are available, the project will determine possible application to Irish conditions. The three distributed catchment models, with different ways of treating spatial information and with different levels of complexity in representing the hydrological fluxes, are being tested. Each of the study catchments represents different climatic and catchment conditions. The models will be compared with empirical, "regression" type models. The reporting of these projects will improve the case work of modeling that is of direct relevance to implementation of the WFD, in particular to the requirements under Articles 4, 5, 8 and 11.

3.3.7. Modelling nutrients and particle transport in lakes

Vollenweider and critical load models for lakes and reservoirs

In the 1970s Vollenweider's models (Vollenweider, 1968; Vollenweider & Kerekes, 1980; OECD, 1982) of nutrient supply and retention in lakes became tenets of limnological thinking and catchment management. Models and management ideas of nutrient load, retention and trophic state are still highly influenced by the thinking of Vollenweider and general relationships between phosphorus loading and standing crops of phytoplankton in lakes (e.g. Dillon & Rigler, 1974). For this reason we describe the fundamentals of the model is some detail. The basic mass-balance model that describes the flow of matter to and from a lake is:

$$V.dC/dt = Q.(C_{in}-C) – R_{sed} . V. C \qquad \text{(equation 3.5)}$$

where

V = lake volume
DC/dt = change concentration per unit time (e.g. yr^{-1})
C = concentration in lake
C_{in} = input concentration
Q = Input discharge (e.g. $m^3\ yr^{-1}$)
R_{sed} =Sedimentation rate (1/time)

The use of this model normally assumes steady-state, assuming conservation of mass, so that $dC/dt = 0$. Lake water retention time (T_w) is the ratio between lake volume (V) and water discharge (Q). The retention of as substance or chemical (T_r) equals T_w if the substance does not change, settle or evaporate once it enters the lake. Considering the open-water of lakes, mostly $T_r < T_w$. The basic model takes this into account by inclusion of a sedimentation factor (Rsed) and solves equation 3.5 at steady state by:

$$C = Q. C_{in} /(Q+ R_{sed} .V) \qquad \text{(equation 3.6)}$$

or $$C = Q. C_{in} /(1+ R_{sed} . T_w) \qquad \text{(equation 3.7)}$$

This basic model developed for the estimation of total phosphorus in lakes (Vollenweider, 1968) generally provides poor estimates (Håkanson & Boulion, 2002) because it does not account for internal loading back into the water column. It is, in any case, difficult to apply because of the need for reliable estimates of, usually costly, estimates of inherently variable river loads, and difficult to measure net sedimentation rates (e.g. Dillon & Rigler, 1974; Larsen & Mercier, 1976). An attempt to address these problems is the use of empirical equations such as that proposed by Vollenweider (OECD, 1982):

$$C=1.55\ (C_{in}/(1+\sqrt{T_w}))^{0.82} \qquad \text{(equation 3.8)}$$

or, proposed for Irish lakes by Foy, (1992):

$$C = 1.118\ C_{in}/(1+\sqrt{T_w})^{1.135} \qquad \text{(equation 3.9)}$$

Approaching the "problem" from the other end these models can be used to estimate substance loads to lakes given a knowledge of mean annual in-lake concentrations. Free (2002) rearranged Foy's model to estimate mean phosphorus loading concentrations for a number of Irish lakes.

$$C_{in} = (C\ (1+\sqrt{T_w})^{1.135})/1.118. \qquad \text{(equation 3.10)}$$

The basic mass-balance equation (3.5) has been reworked by Håkanson and Peters (1995) and represented by Figure 3.9. This allows a visualisation of the dynamics at play, using a software programme such as STELLA to model dynamic systems (Deaton & Winebrake, 1999); Westervelt, 2001). For information on a number of system software packages, including STELLA, see:
http://www.hps-inc.com/science/science.htm.

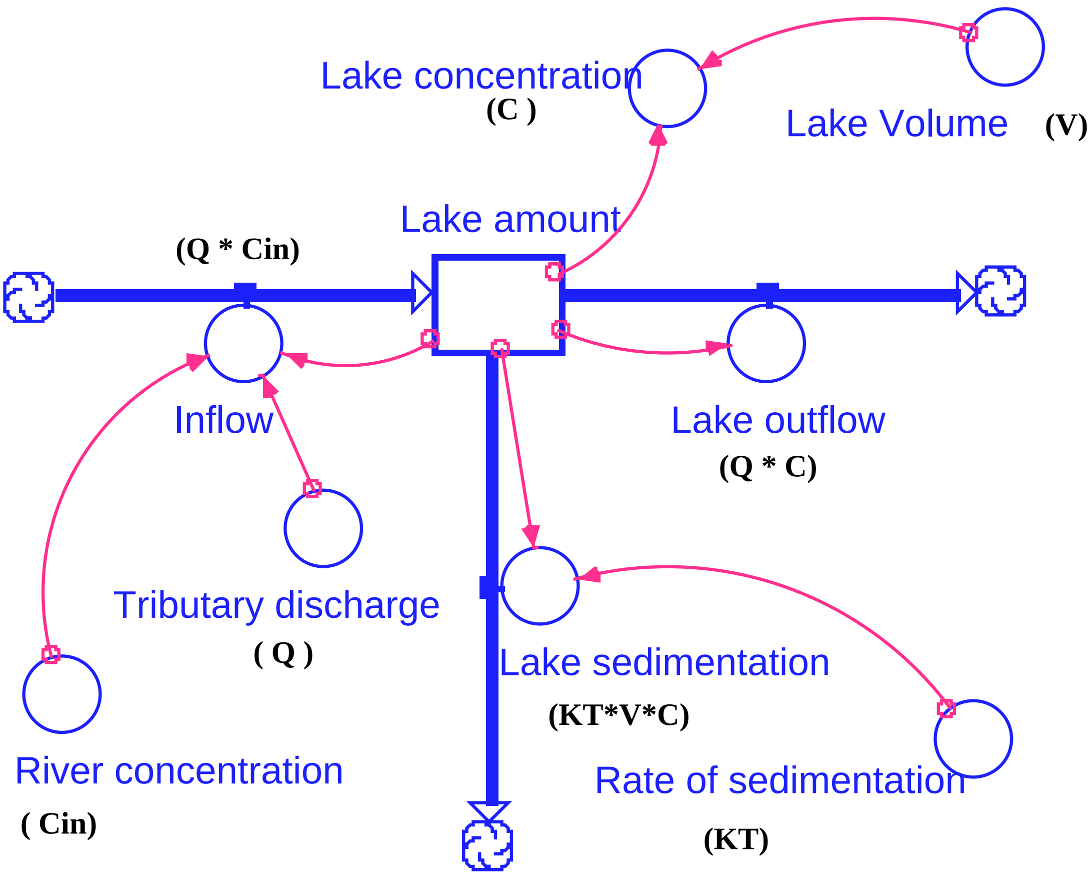


Figure 3.9. Representation of the Vollenweider mass balance equation (equation. 3.5) as a dynamic visualisation, using STELLA (After Håkanson and Peters 1995).

The Vollenweider modelling approach has been used extensively for lake management (e.g. Dillon & Rigler, 1974, Larsen & Mercier, 1976; Reckhow, 1979; Reckhow, & Chapra, 1983). However, such use has been criticised (e.g. Håkanson, 1999; Håkanson & Boulion, 2002) because of the degree that the models simplify, or ignore, the lake dynamics represented in Figure 3.9. Notably, they do not account for seasonal variations, internal loads, or links and feedbacks with the biota. Caveats to the use of the simple Vollenweider approach was emphasised in the original publications (Vollenweider, 1968; OECD, 1982), but are often ignored in lake management. In particular the models do not account for:

- Seasonal variation in phosphorus flux;
- Bioavailability of TP;
- Internal loading of phosphorus; and

- Patterns of phosphorus retention in lake water through seasonal mixing and stratification.

The widespread use of Vollenweider models lies in the critical importance that phosphorus has for the ecology of lakes. Linking phosphorus to ecology, however, requires quantitative relationships between the two. Peters (1986) lists 16 regression equations relating total P to status of separate biotic or abiotic elements in lakes. Further discussion of the modelling of biotic elements for measurement of phosphorus is given in section 3.4.

Examples of "off-the shelf" models for estimation of total phosphorus (and also applicable to N) are EUTROMOD and BATHTUB. In EUTROMOD (Reckhow, 1990), P and N retention parameters are estimated using non-linear regression analysis of regional datasets of US lakes. EUTROMOD predicts median growing-season (June-September) P and N based on annual inputs of P and N. This modelling software also predicts growing-season chlorophyll a and Secchi disc transparency from regional regression models transparency and, through maximum likelihood logistic regression models, estimates seasonal probabilities for blue-green algal dominance and hypolimnetic anoxia. BATHTUB predicts water quality conditions (total phosphorus, total nitrogen, chlorophyll-a, transparency, and hypolimnetic oxygen depletion) using empirical relationships derived from assessments of reservoir data. Ernst *et al.* (1994) considered BATHTUB an effective tool for lake and reservoir water quality assessment and management, particularly where data are limited. BATHTUB is recommended to be used along with two other programs, FLUX and PROFILE for assessments of eutrophication-related processes and effects (see http://www.wes.army.mil/el/elmodels/emiinfo.html). FLUX allows estimation of tributary mass discharges (loadings) from sample concentration data and continuous (e.g., daily) flow records and PROFILE facilitates analysis of in-lake water quality data. Algorithms are included for calculation of hypolimnetic oxygen depletion rates and estimation of area-weighted, surface-layer mean concentrations of nutrients and other eutrophication response variables. All the models discussed in this paragraph were developed for use in the US. BATHTUB, however, may be restricted for use in semi-tropical areas as it was developed for lakes in regions of the southern U.S. All are based on annual steady-state.

Seasonal patterns of TP

Concentrations of total phosphorus measured in surface waters are affected by seasonal patterns of climate, hydromorphology, land-use and biotic transformations. General principles relevant to Irish waters are reviewed in Jennings *et al*. (2003). These factors have major implications for the modelling of phosphorus in surface waters and, more critically, the biotic response to those concentrations. In lakes, internal release of phosphorus from sediments complicate interpretation of mass-balance models, particularly in nutrient enriched lakes prone to stratification (Nürnburg, 1998; Søndergaard *et al.,* 2002). The general practice of mass-balance models to treat the lake as a steady-state reactor tank, summarised in annual increments, inevitably loses important information. Many Irish lakes are, however, prone to summer mixing. Nürnburg (1998) provides a modelling approach applicable across lake types and Håkanson and Peters (1995) suggest that in lakes where summer TP within individual lakes can be highly variable among sampling occasion, winter measurements provide a better, and more cost-effective, sampling strategy. Dillon and Rigler (1974) used spring TP as the predictor of summer chlorophyll a concentrations. Seasonal variation of TP in individual Irish lakes poses major problems for reliable estimation of in-lake conditions estimated from infrequent monitoring (Irvine *et al.*, 2001). Models that address this appear highly beneficial as supporting tools for, at least, lake classification. Existing data sets in Ireland could be used to develop such models.

Mukhopadhyay & Smith (2000) observed, "while it can be argued that, by its very nature, a sparse data set is inconclusive, it must also be acknowledged as frequent reality in the face of resource constraints". With infrequent measurements of nutrient concentrations and discharge rates, there are a number of options for the estimation of total annual or seasonal loads (Dolan *et al*., 1981; Mukhopadhyay & Smith, 2000). The choice of these may depend on the strength of the relationship between flow and nutrient concentration of inflowing streams. If strong, then a ratio estimator (Kendall & Stewart, 1968; Dolan *et al.*, 1981) which takes into account the relationship and variance between daily flow and load from available data in order to provide average loads over defined time period, appears the best option. If the flow-concentration relationship is not strong, a stratified monthly sampling of annual loads will be a better predictors of total load.

While new developments (e.g. Håkanson & Boulion, 2002) permit incorporation of seasonal dynamics within models, it is important to realise it is still widely considered that the use of mass balance models to predict higher resolution spatial or temporal pattern are generally restricted by resource implications of time, money and data. In addition, complex process models such as WASP that are designed to predict dynamic response may, nevertheless, be frequently unreliable (Reckhow, 1990).

Recommendations:

- Vollenweider steady-state models have been used extensively in water management and has application for the prediction of TP from loading estimates. However seasonal variation can be high and this is not addressed in the models. Application is best when applied to specific lakes, rather than as a generic regional model.
- Sparse data sets are often a reality of monitoring and *post priori* modelling. Techniques to deal with these do exist and should be used where applicable in order to strengthen reliability of results.

3.3.8. Modelling Acid status

Acid deposition in areas of low buffering capacity reduces the pH of soils and waters and can cause leaching of aluminium which impacts upon freshwater ecological communities. Waterbodies in Ireland at risk from acidity occur in clusters, in Counties Donegal, Galway, Kerry and Wicklow (Bowman, 1991), and are related to geological occurrence of resistant rocks, particularly granites. Acidification problems in Ireland arise mainly from inappropriate forestry plantations and acid deposition in areas with low background buffering capacity. Owing the prevailing winds, atmospheric deposition in Ireland is generally of a lower overall extent than in other parts of Europe but, nevertheless, may be of local importance (Farrell *et al*., 1997). Reference conditions for acid status can be derived either from a calculation of Acid Neutralising Capacity using empirical relationships with non-marine cations and dissolved organic carbon (Cantrell, Serkiz, & Perdue, 1990; Fozzard *et al*., 1997; Henriksen *et al*., 1992) or, in lakes, from diatom frustules preserved in sediment cores.

A Regional approach to assessment of acid deposition in Europe, and the interface of models and policy has been primarily through The Regional Air Pollution Information Systems (RAINS) (Schöpp *et al.*, 1999). See http://www.iiasa.ac/. An example of a further development of a regional atmospheric transport and deposition model is DAIQUIRI (Deposition Air Quality and Integrated Regional Information) developed by the Finnish Environmental Institute (Syri *et al*., 1998; Kangas and Syri, 2002). Models developed for more widespread application and used for assessing deposition of SOx and NOx applicable to a more local scale include MAGIC (Cosby, *et al*., 1985ab), MAGIC-WAND (Jenkins *et al.*, 1997) MERLIN (Cosby *et al.,* 1985ab) and PROFILE. These have been used to address impact of deposition and are long-term, process-based models used for assessing emission scenarios (Wright, *et al*., 1991), critical loads and impacts of land use change. The MAGIC model has been applied and tested extensively in a number of catchments in many regions of the world has provided a useful modelling tool for understanding catchment processes and guiding management (Cosby *et al.,* 2001). This has included quantifying the role of afforestation as a further casual factor for acid status of surface waters (Wright *et al*., 1994). Recent developments (MAGIC7) of the model (Cosby *et al*., 2001) has linked soil nitrogen and carbon pools to acidification and enabled simulation of short-term episodic responses of mixing fractions of water coming from different pathways.

There is increasing recognition that heterogeneous catchments require a range of modelling approaches, with data collections made at appropriate spatial and temporal scales (Langan *et al*., 1997; Neal, 1997). The difficulties of the application of catchment models at a variety of scales were outlined in section 3.3.2, *'Issues of Scale in hydrological modelling'*. Recent work on acidification models, but also highly applicable to diffuse pollution models and similar to the philosophy adopted by e.g. P –tools (Heathwaite *et al*., 2003) advocates the integration of modelling approaches and scales. An example relevant to the modelling of acidifying impacts on waters is provided by Wade *et al.* (2001). This work combined conservative mixing concepts from a variety of source-pathways, described by End Member Mixing Analysis, EMMA (Christophersen *et al*., 1990) with the MAGIC model, together with multiple regression analysis of catchment characteristics incorporated into a GIS. The models were integrated into a Functional Unit Network (FUN), which divides a river catchment into smaller more homogenous units assumed to be indicative of similar hydrological and biochemical processes (Neal, 1996; 1997 and section 3.3.2, '*Hydrological Response Units'* for associated terminologies).

While there has been much work on the ecological response of freshwaters to acidification (Confer *et al*., 1983; Yan & Strus, 1980; Stenson *et al*., 1993), the ecological response to reductions of acid status remains uncertain. Yan *et al.* (2003) outline the need for model development to help assessment of recovery of surface waters from reduced acid status.

3.3.9 Dangerous substances

The European Water Policy has a legislative history dating back to the early 1970s. Water pollution (see Box. 3.1. for definition) was identified as a priority issue, requiring action by the First Action Programme on the Environment (European Community, 1973). One of the first tasks was to set standards for rivers, lakes and reservoirs used as drinking water sources, reflecting the highly prioritised EU water policy principle to protect human health. Quality objective legislation on fish waters, shellfish waters, bathing waters and groundwaters followed. The main emission control element of the EU Water Policy is the Directive 76/464/EEC on pollution caused by certain dangerous substances discharged into the aquatic environment of the community. The Directive covered discharges to inland surface waters, territorial waters, inland coastal waters and ground water. The protection of groundwater was later moved to a separate Council Directive (80/68/EEC) on protection of groundwater against pollution caused by certain dangerous substances. At the time of its introduction, the Dangerous Substance Directive (76/464/EEC) had to face the challenge of regulating potential aquatic pollution by thousands of chemicals already produced in Europe at that time. The concepts of List I and List II substances (listed in the Annex to the Directive) was adopted. Allocated to List I are certain individual substances which belong to families and groups of substances mainly selected on the basis of their toxicity, persistence and bioaccumulation (e.g. organohalogen compounds, mercury and cadmium and its compounds). List I of the Directive dealing with more dangerous substances and the conditions under which permits may be issued for those substances were regulated in the so called “daughter directives”. List II covers families and groups of substances that have a deleterious effect on the aquatic environment (e.g. metalloids and metal plus their compound, biocides plus their derivates and substances impacting the oxygen balance such as ammonia and nitrites). List II also contains all the individual List I substances that have not yet been regulated on Community level. Less dangerous substances (List II) are subject to pollution reduction programmes in each member state. The basic regulatory principle of the Directive is the licensing of economic activities by the competent national authority. The licence is dependent on emission control on amounts of pollution discharged into the aquatic environment and the overall quality of the aquatic systems. This regulatory approach led to a focus on point source pollution control in Directive 76/464/EEC.

Box 3.1: Definition of pollution in WFD

Pollution is defined as the direct or indirect introduction as a result of human activity, of substances, vibrations, heat or noise into the air, water or land which may be harmful to human health or the quality of the environment, result in damage to material property, or impair or interference with amenities and other legitimate uses of the environment. (Integrated Pollution Prevention and Control Directive 96/61/EEC).

A second phase of water legislation arrived after the Frankfurt Ministerial Seminar in 1988 with the revision of the water policy. The Urban Waste Water Treatment Directive (91/271/EEC) was put into place to provide an even more stringent biological treatment of waste water. The Nitrates Directive (91/676/EEC) complemented the Urban Waste Water Treatment Directive by addressing directly the problem of nitrate pollution of water from agriculture. Both Directives combine the quality objectives and emission limit approach to obtain pollution control. Other legislative results of the Seminar were Commission proposals for action on a new Drinking Water Directive and the Directive for Integrated Pollution and Prevention Control (96/61/EEC).

A further ministerial meeting on Water Policy in The Hague (1991) proposed a Programme for the protection and management of groundwater (Groundwater Action Programme European Communities, 1996). The Ecological Quality of Water Directive (COM (93) 68) was proposed to complement the Groundwater Programme and the main objective was to maintain and improve quality of surface waters by requiring member states to monitor the ecological status, identifying potential sources of pollution, and establish targets and programmes for achieving good ecological status in water. The Fifth Action Programme on the Environment (European Communities, 1993) set out the objectives for water quality and quantity until the year 2000. The quantity objectives dealt mainly with the sustainable use of the fresh water resource. The quality objectives for groundwater were maintenance of unpolluted sources, prevention of further contamination of already polluted groundwater and the restoration of contaminated groundwater to drinking water quality. Quality of surface water was to be established by the maintenance of high ecological quality with high level of biodiversity. Marine water quality was assured by the reduction of discharges of toxic substances that have harmful, persistent and bioaccumulative characteristics.

The high number of Water Policy Directives unfortunately fragmented the objectives and reduced the effectiveness of the Water Policy. In 1994 the European Environment Agency reported that only 10 percent of EU river and lake water fulfilled the EEA's criteria for good water quality (Grant, Matthews and Newell, 2000). The proposal of a Water Framework Directive was presented in 1997 to provide an integrated framework to protect surface water, groundwater, estuaries and coastal waters together. The WFD (2000/60/EC) rationalises and updates existing water legislation by setting EU wide objectives. The key aims of the WFD are the provision of drinking water and other economic activities, the protection of the environment and the alleviation of the impact of floods and droughts. The river basin management system is used where each district provides the primary administrative unit for coordinating implementation of the Directive under the designated competent national authorities. The Framework Directive is a new integrative approach to water pollution control and the River Basin System takes the flow of water through the aquatic system into account, an improvement to the static nature of categorised water compartments used in the early Directives. The WFD lays out a requirement for ecological protection and minimum chemical standard for surface waters. Annex V of the WFD defines the required "*good ecological status*" in terms of quality of the biological community, the hydrological and chemical characteristics. "*Good chemical status*" is defined in terms of compliance with all the quality standards outlined for chemical substances at EU level. The WFD advocates a precautionary approach to define the chemical status for groundwater since it should not be polluted at all. There is generally a prohibition on direct polluting discharge to groundwater and additionally a requirement to monitor groundwater for detection of potential changes in chemical composition of groundwater.

The strategy against pollution of water in the WFD requires a list of "priority substances" that contains "hazardous substances" (Box. 3.2. for definitions) presenting a risk to the aquatic environment. A legal framework and a clear prioritisation of substances was laid down in Article 16 of the WFD. The Combined Monitoring-based and Modelling-based Priority Setting (COMMPS) procedure was developed and applied in the selection process of the proposed priority substances. In the application of

COMMPS procedure about 820,000 water and sediment data from all Member States were evaluated. Data of more than 310 substances produced and used in Europe were used for modelling if the available monitoring information was insufficient. As a result of the COMMPS study 32 substances or groups of substances were identified for the list of priority substances. The main purpose of the Dangerous Substance Directive was emission control by elimination or reduction of certain pollutants stated in List I and List II, respectively. Only 18 substances of 132 proposed List I substances, have been regulated on Community level as “List I dangerous substances” under the “Daughter Directives” since the Dangerous Substance Directive was put into place in 1976. Some substances of List I were added to the Priority Substance List of the WFD, indicating that pollution has not been eliminated. Under the WFD the Dangerous Substance Directive will be repealed and a review of all Daughter Directives was required within 2 years after enforcement of the framework. The Priority List of the WFD will replace List I of the Dangerous Substance Directive (76/464/EEC).

Box 3.2: Definition of Hazardous substances *and* Priority substances in WFD

Hazardous substances -

means substances or groups of substances that are toxic, persistent and liable to bio-accumulate; and other substances or group of substances which give rise to an equivalent level of concern (Article 2, ‘29 in WFD).

Priority substances –

means substances identified in accordance with Article 16 (2) and listed in Annex X. Amongst these substances there are *priority hazardous substances* which means substances identified in accordance with Article 16 (3) and (6) for which measures have to be taken in accordance with Article 16 (1) and (8) (Article 2, ‘30 in WFD).

Despite the new approach, the framework still faces the problem of the continuous increase of suspected dangerous substances and the potential effect of a “cocktail” of these substances mixed together in the water. The modelling of selected dangerous substances to test and finally predict their impact on the ecosystem and human health is very difficult to generalise because of the very same reason. Interactions between chemical substances and different ecological, geological, physico-chemical habitat structures make the transformation of data difficult. The number of monitored and modelled substances appears small in comparison with the high number of chemical substances present in the aquatic system. A current EU project REBECCA (http://www.environment.fi/syke/rebecca) is investigating the link between ecological status and chemical status of surface waters.

Recommendations: Computer models that analyse dangerous substances in aquatic systems are often very specific (e.g. formation of POX and NPOX with chlorination of fulvic acid in water: empirical models (Zou et al., 1997)) to the compound in question and habitat parameters. The use of such models in Ireland should be done with care. The chemical status and other habitat conditions (e.g. hydromorphology) of the Irish water body have to be comparable to the modelled situation and potential synergistic effects with other chemical substances present in the water have to be taken into account.

3.4. State-Impact models

3.4.1. Introduction

The WFD requires classification of water bodies based on departure from a minimally impacted state. It also requires that the indicators of that change are, primarily, the biota. This is, in general, a departure from the heretofore emphasis on chemical determinants as metrics of quality. This shift in policy presents major challenges within the timeframe of the first phase of the WFD. Characterisation of water bodies, among which biotic response to Pressures will vary, is required by 2004, as too does it appear there is a need for a preliminary definition of reference state, although the obvious need for periodic review of these is recognised within the text of the WFD. Monitoring systems need to be in place by 2006. By and large, reference conditions for many biotic elements are unknown and response of biota to pollutants can be highly variable among waterbodies and seasonally. Spatial heterogeneity is a feature of the natural world and needs to be incorporated into monitoring and reporting protocols. In the midst of all this uncertainty, application of appropriate mathematical models can play an important role to help meet the requirements of the WFD. However, if uncertainty that affects monitoring and analytical procedures are not properly addressed in the application of models, there is a high risk that the use of models will serve no purpose other than to obfuscate reporting requirements. The use of models to simulate patterns of the biota and their response to increase or decrease in Pressures needs, therefore to be carefully thought through and with clear aims and objectives prior to their use. This section reviews a number of modelling options to help describe and predict impact from pollutants on receiving waters. It is, however, worth bearing in mind the opinion of Håkanson and Peters (1995) that “extensive ecosystem models where all rates and model variables are empirically calibrated for a given lake might provide the best predictions in that lake, but they usually fail in other lakes”. The message is a clear one with respect to the WFD. If the complexities of ecological systems means that we cannot, without intensive effort, model all the factors that we think are important for structure and biological functioning of surface waters, it is imperative that the questions we do ask are appropriate to relatively simple monitoring; or of a general enough nature to be applicable at least within defined typologies. The challenge of the requirements of the WFD is to identify reliable indicators of ecological quality and, as required, direct the modelling effort towards them rather than adopting a broad approach in the hope of successful *post priori* modelling.

3.4.2. Effect-Load-Sensitivity (ELS) Models

To understand impact of a pollutant, and to effect management to reduce pollutant loads that are widely accepted, it is necessary to demonstrate reliable dose-response relationships. This drives the determination of Effect-Load-Sensitivity (ELS) models and the subsequent determination of *Critical Loads* and management of *Maximal Allowable Loads*. Such concepts drive water quality monitoring programmes required under the U.S. Clean Water Act (section 3.4.5). These principles are also of fundamental importance for the implementation of *Programmes of Measures* within River Basin Districts under Article 11 of the WFD. For some pollutants, such as heavy metals and pesticides, the determination of maximum allowable loads is typically circumvented through the measurement of *Maximum Allowable Concentrations* in the receiving waters or within indictor organisms, typically top predators. This approach is used quite effectively in the implementation of some current Directives (e.g. 75/440/EEC, 76/464/EEC, 80/68/EEC, 98/83/EC) that address directly risk to human health. Acceptible thresholds for ecological health are much more difficult to define as the load-response relationship is often highly uncertain and, in addition, variable among water bodies. The very concept of *Programmes of Measures* requires reliable estimates of the effect of pollutant loads on ecological status or, and more likely possible, indicators of ecological status.

Measures of ecological status, as defined within the WFD, relates to ecological and not load variables. Practical and effective ELS models need (after Håkanson, 2001) to:

- be characterised by a relevant and simple structure, involving the smallest possible number of driving variables;
- use driving variables that are easy to measure; and
- are able to be validated for a wide range of circumstances across a variety of environmental characteristics.

In water bodies this last requirement does not negate the use of models applied to systems with variable sensitivity (e.g. impact of acid deposition on lakes of varying alkalinity), but it does require that it is possible to identify broad categories of water-body types (as indeed stated in Annex II of the WFD) with similar sensitivities.

In lakes, the most common documented response of ecological elements to nutrient loads has been that of the phytoplankton (Dillon & Rigler, 1974; Schinder, 1978). This is reflected in the many current lake classification schemes (e.g. DELG, 1998) based on the original OCED (1982) trophic divisions. The fixed boundaries of such schemes take scant heed of either seasonal variations (of both lakes and sampling regimes (Irvine *et al.*, 2002) or different responses of the chlorophyll a: total phosphorus relationship across lakes types (Hessen *et al.*, 1992; Andersen, 1997) driven by e.g variations in lake colour (for Irish lakes see (Irvine *et al.*, 2001)) and physical/biotic structure (Scheffer, 1998). Implementation of the WFD certainly requires further development of ELS models in relation to nutrients and their impacts on a range of biotic elements. Lessons in achieving this can be learnt from the experience in the U.S. of managing surface waters on a basis of allowable Total Maximum Daily Loads, discussed futher in section 3.4.5.

Critical load models for acidity (Cantrell *et al.*, 1990; Henriksen *et al.*, 1992) have been adopted in e.g. monitoring strategies in Scotland (Fozzard *et al.*, 1997) and Sweden (Fozzard *et al.*, 1997; EPA, 2000; SwedishEPA, 2000). Acid neutralising capacity is compared with estimated reference values of pre-industrial levels based on empirical relationships (Cantrell *et al.*, 1990). Alternative methods for estimation of reference state of aciditity is through use of transfer functions that relate pH to sediment characteristics assessed by paleolimnological techniques. Typically such work has relied on assessment of ELS using diatom remains (section 3.4.3, palaeolimnology), although recent work has opened up the possibilities for a whole array of remains in the sediments of lakes to be used in models that assess historical changes through contemporary sampling.

While work relating chemical conditions in water to aquatic life has a long history through e.g. toxicological studies for listed substances, prevalence of macroinvetebrates in relation to oxygen state in rivers and the examples given above, current demands of the WFD require more detailed understanding of the link between chemical and ecological status. This is likely to be developed by one of the “second round” Common Implementation Strategy Group, ECOSTAT. This is a future area where modelling will be highly applicable and where a new E.U. funded project, REBECCA which will study the relationships between ecological and chemical status of surface waters, is likely to be useful.

Recommendations: ELS models relate sensitivity of biotic elements to chemical status. This is fundamental to the assessment of risk to failure to meet Environmental Objectives. Modelling within such studies have and will continue to be important for assessment of the relationship between ecological and chemical status of waters. Understanding of these relationships, relevant to all biotic elements, can be furthered through literature collations, awareness of ongoing current work and, where necessary, focussed new work.

3.4.3. Lakes and Rivers

Modelling the chlorophyll-TP response in lakes

Vollenweider-type models predict TP as a response variable to lake loads. However, lake management is concerned ultimately with the biological response to State variables such as phosphorus (State-Impact in the DPSIR framework); and this is clearly the philosophy adopted by the WFD and drives the classification of water bodies, as outlined in Annex V of the WFD. Håkanson and Peters (1995) draw the important distinction between *limnological state variables* such as TP and *ecological effect variables* such as phytoplankton chlorophyll *a*. The usefulness of knowledge of state variables is only realised by the relationship between chemical and ecological status (see ELS model discussion above). Indeed this applies to all biotic response-chemical load scenarios which describe the relationship between the State and Impact in the DPSIR model described in Chapter 1**.** In lakes, the main focus has been on the TP-chlorophyll *a* relationship (Dillon & Rigler, 1974) and models that help understand, quantify or predict that relationship are clearly of importance in the implementation of the WFD.

The response of phytoplankton (usually measured as chlorophyll-a, but required under the WFD to include consideration of net cell volume of phytoplankton) to given concentrations of TP is variable, both among lakes (Faafeng *et al.*, 1990; Hessen *et al.*, 1992; Andersen, 1997; Håkanson, 1999) and within years. Significant spatial variability within a lake is also possible. If predicting TP loads to a lake makes Vollenweider model application a uncertain endeavour, the added error in prediction of phytoplankton response to ambient nutrients does not bode well for application of these models to implementation of the WFD. Håkanson & Boulion (2002) address these concerns in the development of a generalised *Lakeweb* model (see below), by linking biotic and abiotic compartments and using small, weekly, time increments. Sub-annual time increments to the modelling of lakes is especially important for predictions of phytoplankton production and standing biomass (see also Håkanson & Boulion, 2003).

Standard water models usually address a single phytoplankton compartment, typically a measure of total phytoplankton biomass, whereas a more useful question relates to the point at which e.g increased nutrient loads lead to a shift to increasing dominance of undesirable species, notably blue-greens (Reckhow & Chapra, 1999). Models have, however, also been developed to predict and understand species dynamics within phytoplankton communities. An example of a major effort has been work on Lake Ladoga, the largest European freshwater lake, and the modelling of phytoplankton succession in response to changes in anthropogenic inputs of phosphorus (Rukhovets *et al.*, 2003). This work has involved extensive effort over many years, with the goal to provide precise information on the response of phytoplankton to internal processes, in order to help with management of the catchment area.

A multiple regression time series model used by Stronge *et al.* (1998) explained 76% of annual variation of spring chlorophyll a concentrations in Lough Neagh, from a dataset than spanned 1974-1992. The important variables in the model were previous year's spring chlorophyll a, SRP April-June and particulate P of the previous summer. This type of modelling can be useful in providing a risk assessment to decline in water quality.

Recent development by U.K. Centre of Ecology and Hydrology to simulate *in situ* dynamics of phytoplankton in lakes, reservoirs and rivers has led to the development of the PROTECH family of models. Simulation of the growth and loss of phytoplankton in natural lakes has been successful and the models are sensitive to the effect of season, nutrient supply, grazing and wash-out losses (Elliott *et al.*, 2001; Reynolds, *et al.*, 2001; Elliott *et al.*, 2002)**.** The models also address changes in community composition of the main phytoplankton species and as such would appear suitable as a tool to address this requirement of the WFD outlined in Annex V. Given initial starting conditions the models predict development of phytoplankton based on laboratory validated growth response. PROTECH has also been used successfully to simulate phytoplankton populations in an Australian reservoir, including incorporation of management techniques, $CuSO_4$ dosing and aeration (Lewis *et al.*, 2002). Other models used to predict chlorophyll *a*, or other indicators of eutrophication such as hypolimnetic deoxygenation, include WASP5, EUTROMOD, BATHTUB and CE-QUAL-W2. Limitations to use include lack of seasonal or spatial resolution and incorporation of temperature dependency. These models are, however, included in the US EPA tool box for lake management (US EPA, 1999). The need for site-specific detailed calibration has generally restricted use of process-type models for prediction of algal response to nutrients. Developments to make these models more generally applicable include DYRESM (Imberger & Patterson, 1981) designed for reservoirs, and to be calibration free. Its applicability has been tested in a number of situations (Imberger & Patterson, 1990). Further developments of this model (Hamilton & Schladow, 1997; Schladow & Hamilton, 1997) couple hydrodynamic and water quality elements to ecological algorithms, which do need calibration. Application of such models has not yet occurred in Ireland but merit consideration for some of the higher profile eutrophicated lakes such as Loughs Leane, Conn and Sheelin.

Recommendations: Simple Vollenweider and multiple regression models to predict response of algae populations in lakes to changes in nutrient loads could be applied without undue difficulty, given estimates of loads and hydromorphology. More complicated process models could be used for some lakes to guide programmes of measures where these are required. In particular, these models should be considered for higher profile lakes where lack of understanding of details of the processes and seasonal dynamics hinder management.

Colour

Humic substances leaching from land and decomposition of aquatic organisms, notably vegetation, imparts colour to water. Although present in all natural waters, concentrations are usually highest in waters draining organic-rich and waterlogged soils. Vegetation cover can also be important, with e.g. drainage from coniferous stands leaching more humic substances than broadleaf forests (Driscol *et al.*, 1988). As rates of decomposition are temperature dependent, so too is export of colour (Kortelainen, 1999). The relationship between colour in surface waters and catchment characteristics is discussed in e.g. Rasmussen *et al.* (1989); Kortelainen (1993) and Hope *et al.* (1994). Additionally, coloured lakes are typically in catchments that release low amounts of base cations and, as such, are vulnerable to acidification. Coloured lakes are typically situated in catchments dominated by peat and peat erosion, and exposure through e.g. over grazing can result in enhanced colour emission from land to water. Colour in water affects light transmission and nutrient dynamics. While this physical effect has implications for biotic response to nutrient supply, the complex chemical compositions in humic waters can also affect nutrient fluxes (Peterson, 1991).

The importance of peatlands in the Irish landscape, of about 20% of land cover, is similar to that of Alaska, Norway and Indonesia. Only in Finland is there a substantially greater proportion of peatland (Kivinen *et al.*, 1979). Range of colour in 200 Irish lakes found by Irvine *et al.* (2001) was 5-174 mg l^{-1} PtCo. A marked seasonal pattern, strongly influenced by retention time, was found in some lakes. Techniques for the modelling of colour is, therefore, important for River Basin Management in Ireland. Håkanson and Peters (1995) provides useful discussion on salient aspects for the modelling of colour in lakes and provides summary of some empirical regressions relating catchment features with lake colour.

The overall concentration of water colour/DOC produced by different catchments is predominantly a function of the amount of peat (Mitchell and McDonald, 1995; Hope *et al*., 1997; Aitkenhead *et al*., 1999). Conceptual models that simulate the export of colour/dissolved organic carbon (DOC) in peaty upland catchments have been developed in the UK (Naden, 1991; Eatherall *et al*., 1998; Naden and Watts, 1998; Naden *et al.*, 2001). Current work in Ireland by N. Allott and E. Jennings (Centre for the Environment, Trinity College, Dublin) suggests that the GWLF model can be useful for predicting seasonal changes in colour, and nutrient inputs, of Irish lakes.

Recommendations: Because colour is likely to affect the nutrient-algae response in many Irish lakes, this should be taken into consideration in modelling work. This will also help develop understanding of the ecological mechanisms in coloured lakes.

Macrophytes

A range of variables are important predictors for distribution of submerged aquatic plants, commonly referred to as macrophytes (Barendregt & Bio, 2003). Light, nutrients, water chemistry, sediment composition and ambient, and variations in, hydrology are important. The extent of depth of colonisation is related to light penetration and hence, all factors that limit light; notably turbidity, colour and phytoplankton standing crop. This response of macrophyte communities to nutrient status has encouraged classification of trophic status of freshwaters based on their submerged plant communities (Spence, 1967; Seddon, 1972; Haslam *et al.*, 1975; Ratcliffe, 1977; Canfield *et al.*, 1983). At high standing crops of phytoplankton, usually fuelled by nutrients, submerged plants may disappear altogether; although alterations in the shift between phytoplankton and submerged plant dominance can occur in, particularly shallow, lakes at moderate-high nutrient enrichment (Scheffer, 1998; and see below). Macrophytes species richness is also responsive to pH, declining with increasing acidity (Jackson & Charles, 1988). At very low pH (<5) there can be widespread loss of angiosperms with increasing dominance by *Sphagnum*. Hydromorphological changes, effected through e.g. land drainage schemes can alter the extent, and nature, of macrophyte coverage, and changes in sediment load can affect turbidity and, hence, the euphotic zone. Macrophytes have also been used to classify lakes for conservation status (NCC. 1989; Palmer, 1989; Palmer *et al.*, 1992). Palmer *et al.* (1992) used multivariate models to identify community types and their relationships with conductivity and hardness. This model is, however, often misconstrued as a classification useful for assessment of nutrient status. A survey in Northern Ireland (Wolfe-Murphy *et al.*, 1992) of 338 randomly selected lakes followed the methods of Palmer *et al.* (1992). In Sweden, macophytes are included in the protocol for assessment of lake water quality (SWEPA, 2000). The presence of extensive macrophyte beds can significantly affect the application of Vollenweider-type models to lakes and cause an underestimation of actual loading in lakes with dense macrophytes owing to nutrient uptake by plants (Berg, 1990).

Charophytes are typical of clear water, calcareous lakes, although they also occur in more acidic conditions. They may also be susceptible to decline during the early stages of eutrophication and any changes in their distribution within a lake is likely to signal increases in nutrient loading (Moss, 1983; Jupp & Spence, 1977;). Increased occurrence of tall ranking plants, such as *Myriophyllum* and *Elodea* species are also useful indicators of increased lake productivity.

Annex V of the WFD requires that macrophytes and other phytobenthos be used for the classification of surface waters. General models for predicting macrophyte distribution and community structure are not well developed, although there has been extensive work on studying the effects of pressures, particularly nutrients, on macrophyte communities in lakes (Jeppesen *et al.*, 1999) and rivers (Bornette & Amoros, 1991; Higler, 1993; Schneiders *et al.*, 1999; Riis *et al.*, 2000). While there is also a long history of work on the relationship between environmental variables and macrophytes (see Carr *et al.*, (1997) for review), there has not been extensive development of mathematical models for the prediction of *in situ* response of macrophytes to changes in driving variables. One attempt to do this for rivers this has been the "Kennet Model" (Wade *et al.*, 2001). Based on a conceptual model of Ham *et al.* (1981) that identified discharge, solar radiation, dredging and shading of epiphytes as the most important controlling factors for macrophtye growth, the Kennet model simulates major stores of P and in-stream processes in the river. It operates on a daily time step. It includes a general sensitivity analysis using Monte Carlo simulations to identify the key parameters controlling model behaviour. The model provides a useful framework for development of generic models that would predict macrophyte growth, but is designed for applicability to lowland chalk streams, with defined boundaries for the ambient physical and chemical boundaries. Other modelling work (e.g. Asaeda *et al*., 2000) has demonstrated the importance of macrophytes for uptake and retention of phosphorus during their growing season and potential for removal of P by harvesting plants at the end of the season. Macrophytes, as important components in many ecosystems, are included in discussion of ecosystem models below.

Lack of robustness of linear models developed to relate macrophyte data collected in the Rivers Test and Itchen in the U.K., led Dawson *et al.* (2000) to explore the usefulness of artificial neural networks to model macrophyte, particularly *Ranunculus,* presence. The authors concluded that such inductive learning models are well suited to handle data that is non-linear, noisy and inconsistent. Artificial

Intelligence models are discussed further in Chapter 4. As both catchment characteristics, and local conditions acting on individual plants are important predictors of macrophyte species composition (Barendregt & Bio, 2003), modelling of state-impact response requires data collections and model construction at both of those scales. Modelling across river basins may also need to incorporate considerations of biogeography, although this is probably not an important issue in Ireland. Recent work at the University of Ulster (B. Rippey, pers com.) is developing predictive models, through use of multivariate statistical techniques, designed specifically to meet the needs of classification of lakes, as required by the WFD.

Macrophyte distributions can be mapped by remote sensing and algorithms applied within GIS to estimate relationships between driving variables, such as sedimentation rates, colour or hydrological regime and to predict changes in response to changes in those variables. Cartographic models within GIS (Tomlin, 1990) provide sequences of GIS data layers, linked by mathematical relationships. Cartographic models also enable interrogation of data and exploration of predictive scenarios. Application of GIS mapping, analyses and modelling techniques provides important potential for assessment response of aquatic vegetation to changes in pressures and for exploring management options (Remillard & Welch, 1993). The potential extends well beyond mapping macrophytes and could be applied for widespread relationships within the catchments. Such models are currently not well developed but are likely to be powerful tools to assist with identification of pressures-impacts and for development and monitoring of *Programmes of Measures* required by the WFD.

Periphyton

Benthic algal communities have been used to assess environmental conditions and the ecological integrity of streams and rivers for over 50 years (Stevenson and Smol, 2003) with metrics developed that include biomass, metabolism, diversity, saprobien-based indicators, mutlivariate analyses, biotic indices, and reference-site based models (Chessman *et al.*, 1999; Lowe & Pan, 1999; Stevenson & Smol, 2003 and Stevenson & Bahls, 1999), the application to routine assessment is still fairly limited. Development of conceptual models of the response to ecological factors e.g. (Stevenson, 1997) provides a foundation of such models and recent research, both in Ireland (De Nicola *et al*., 2003; 2004) and elsewhere (King *et al.*, 2000; Seele, 2000; Schönfelder, 2002) illustrates progress for use of benthic algae models for the assessment of lakes. Use of diatoms can aid river monitoring schemes (e.g. Kelly & Whitton, 1995; Eloranta & Kwandrans, 2000).

Developing predictive relationships between environmental conditions and periphyton (Horner *et al.*, 1990) is, however, a difficult challenge (USEPA, 1999), complicated further by factors such as high local and diel variability of dissolved oxygen cycles among periphyton (and macrophyte) mats (Butcher & Covington, 1995) and catastrophic loss of algae during spate conditions (Uehlinger *et al.*, 1996). A study to assess effects of nutrient enrichment on development of benthic algal mats in rivers, (Dodds *et al.*, 1997) using a stepwise regression model from an extensive data set collected from Europe, the US and New Zealand, found that greatest amount of variance in benthic chlorophyll *a* was accounted for by TN, followed by TP. However, predictive power was low (best fit $r^2 < 0.43$). An alternative model (after Heiskary & Walker, 1988) that predicted probability of exceedence of a user defined measure of disirable quality (set at critical values of 50, 100 and 150 mg chl *a* m^{-2}) also revealed a clearer relationship between chlorophyll *a* and TN than with TP Dodds *et al.*, (1997) found no relationship between TN:TP ratio and *Cladophora* abundance and concluded it difficult to predict impact of nutrient management on *Cladophora* growth. Further work in New Zealand streams by Biggs (2000) concluded that frequency of maxima of algae areal biomass was best explained by average time between spate flows.

Welch *et al.* (1992) developed a model based on laboratory response of periphyton to predict its biomass on natural substrata at 26 sites above and below point source discharges in 7 New Zealand streams. While point-source enrichment increased biomass substantially at the majority of enriched sites, overall, biomass averaged only 35%, and with high variation, of the concentrations predicted from phosphorus, velocity and temperature using the model. Furthermore, aesthetically nuisance biomass levels (i.e. > 200 mg chl *a* m^{-2}) were observed at only 7 of 19 enriched sites. In many cases, the lower than expected biomass levels were attributed to high macroinvertebrate grazer densities, riparian shading or unsuitable attachment surfaces.

Recommendations: The potential for using robust models, at least within the short-term, to predict periphyton biomass in rivers is uncertain. The situation in standing waters would seem no better. Complex ecological interactions among components of the phytomacrobenthos (macrophytes, epiphytes and epibenthos), the phytoplankton, littoral invertebrates and zooplankton (Phillips *et al.,* 1978; Underwood, 1991; Daldorph & Thomas, 1995; Scheffer, 1998) act against widely applicable use of mathematical models to help with WFD implementation. Models developed for specific sites may be more feasible, but of limited use at regional or River Basin scales. Site specific models in Ireland require further research, although development of simple regression models linking periphyton with physical and chemical variables would be a relatively simple, and perhaps useful, endeavour.

Macroinvertebrates

The use of macroinvertebrates as indicators of river quality has a long history (see reviews in Hellawell, 1986; Metcalfe, 1989). Monitoring schemes such as the Trent Biotic Index (Woodiwiss, 1964) and that of the Biological Monitoring Working Party (Chesters, 1980) were adapted by An Foras Forbartha into a national monitoring programme of Irish rivers that has existed since 1972 (Flanagan and Toner, 1975). This evolved into the current three-year rolling programme coordinated and operated by the EPA. In this programme water quality is assessed by the derivation of a biotic parameter (the Q-value) based on invertebrate community composition, with subsidiary information on chemical variables (Lucey *et al*., 1999). Although the original biotic schemes for rivers were developed to measure invertebrate community response to organic loads and decline in oxygen concentrations, the Irish EPA has effectively used this scheme as a surrogate metric of phosphorus loads. In rivers where acidity is considered to be the main problem greater reliance has been placed on chemical rather than biological assessment (e.g. Bowman, 1991; Allott *et al*., 1997). The Q-value scheme is simple to apply and based on a scoring system that reflects invertebrate tolerance to pollution, although there is a risk in inexperienced operators of inconsistency in its application. The scheme also compares among rather than within sites. As such, it is not designed to take into account reference conditions as defined in Annex V of the Water Framework Directive. In practice, the benchmark of the Q-value is that of well-aerated streams with moderate to high flow regimes. Current work in Ireland led by the Central Fisheries Board is attempting to relate Q-value with fish population structure in rivers.

The USEPA has adopted widely the use of models for the classification of river water quality. These use a variety of metrics that cover an array of biological groups that, when integrated, provide an overall assessment of quality. Such a multimetric approach to bioassessment is used by more than 90% of state agencies in the U.S. (Barbour & Yoder, 2000). The approach is detailed in Technical Guidance Documents (USEPA, 1998). Biological Integrity in surface waters is estimated relative to reference conditions and results of monitoring are communicated in a manner understood by water managers and the general public. The biometric approach includes criteria for reducing the number of metrics to the most relevant core group to be aggregated into a single quality score. This score provides information on whether action (programme of measures) is required, but the nature of that action is determined by further analysis of the component metrics. Commonly used biometric models are described by Karr *et al.* (1986), MacCormick *et al.* (2000), Barbour *et al.* (2000) and Paulson *et al.* (1998). The multimetric approach is, however, not without its critics. Resh *et al.* (2000) reported that multimetric assessment can provide a low predictability of correctly assessing impairment of a site and that metrics based on taxa richness were less prone to error than more complicated parameters that incorporated measures of abundance. Resh *et al.* (2000) recommended that multimetric assessment would benefit from incorporating multivariate approaches.

Unlike the multimetric approach, establishing reference conditions by multivariate analysis makes no a priori assumptions of community similarities based on physico-chemistry (Reynoldson *et al.*, 1997). Sites are grouped based on biotic composition, with an assumption that biotic composition reflects the ecological drivers that configure the community. Multivariate models that assesses ecological quality, by comparison with a defined reference state, include the U.K RIVPACS (River InVertebrate Prediction And Classification System), AUSRIVAS (AUStralian RIVer Assessment Scheme models) and, in lakes, BEAST (BEnthic Assessment of SedimenT).

RIVPACS, now at version III and, developed over three decades in England, Scotland, Wales and Northern Ireland, uses species data and log10 categories of abundance of families to assign reference communities to one of 35 groups, using TWINSPAN (Wright, 2000). These groups do not necessarily define typology as defined by Annex II of the Water Framework Directive, but could clearly be used in the verification of typology based on categorisation of catchments. Communities are sampled by standard methods, with site weighting to reflect proportional habitat and communities related to (in U.K.) twelve environmental variables Test of assignment of 614 reference sites were correct for 51.6% of sites, and for second highest probability for correctness of fit, 18.1% (Wright,, 2000). Classification of operational sites predicts the probability of occurrence of taxa in the absence of environmental stress. Algorithms that compare ‘observed’ with ‘predicted’ estimates site quality. The model can be run for various probability thresholds and to model likelihood of occurrence of taxa, BMWP family predictions or abundance of sensitive taxa. The model, while successful as a descriptor, or for classification relative to reference state, of invertebrate communities, appears a poor predictor of pollution-driven future alterations to communities, even of those that involve changes to the habitat (Armitage, 2000). This was, however, never a goal of RIVPACS, but a useful future development of the model would be to develop such a capability. Recent reviews of the model and its application can be found in Wright, *et al.* (1998) and Wright *et al.* (2000) and a comparison with other predictive techniques of river invertebrates in Moss *et al.* (1999). Johnson, & Sandin (2001) report on the development of a RIVPACS type approach for prediction and classification for invertebrates in the littoral of lakes and riffle areas of streams in Sweden.

AUSRIVAS (Smith, *et al.*, 1999; Turak *et al.*, 1999) was developed from the concepts of RIVPACS. Differences include: the sampling of, and model application to, separate habitats; twice (as opposed to thrice) yearly sampling; for the most part, identification of invertebrates not beyond the family level; alternative multivariate techniques; and use of an Australian analogue of the average score per taxon (ASPT) rather than the BMWP-type metrics (total score, total scoring taxon number and ASPT) used in RIVPACS (Wright, , 2000). The model has, and continues to be, incorporated into state environmental policy and monitoring protocols and set to develop into an integrated river assessment package (Davies, 2000). The manual for model use can be downloaded from:
http://ausrivas.canberra.edu.au/Bioassessment/Macroinvertebrates/Man/Pred/.
Use of the software costs currently Aus $80. It comes with the disclaimer, appropriate to such models, that “AUSRIVAS is a predictive model. Predictive models by their nature have the potential to provide incorrect predictions and should not be relied on”. It is being further developed for fish and diatoms. In New Zealand, a similar approach to predict the effect on fish and crayfish communities from building of dams has been reported by Joy & Death (2001).

BEAST is a multivariate statistical approach that was developed to compare lake benthic communities in impacted and unimpacted sites in the Laurentian Great lakes (Reynoldson, 1994; Reynoldson *et al.*, 2000) but has also been tested in rivers (Reynoldson *et al.*, 1997; Rosenberg *et al.*, 2000). The model tests a site against only those reference sites to which the test site is predicted, whereas RIVPACS and

AUSRIVAS compares the test site with all reference sites, applying a probability weighting (Reynoldson *et al.*, 1997). In a comparison of multimetric and multivariate approaches, Reynoldson *et al.* (1997) outlined strengths and weaknesses of AUSRIVAS and BEAST and recommended that both methods could be usefully employed. It was considered that multivariate models were generally more powerful than multimetric ones, although the later had the advantage of producing a single value that appeals to managers, and which is easy to communicate to a non-technical audience. More information about BEAST is available at http://www.nwri.ca/cgi-bin/mfs/01/nwri/issues/cabin/beast-e.html

While the RIVPACs type approach is gaining in popularity and application, there may be inherent weaknesses that undermine its ability to make maximal use of the information contained within the field data. These systems typically include a model that predicts the 'unpolluted' reference community of 'polluted' sites, and then classifies them on the basis of two or more ratios of selected properties of the 'polluted' and reference communities. Very little use is, however, made of the wealth of information contained in the extensive databases of routinely recorded field data. Instead, the main model is based on a relatively small set of pre-selected reference sites, which may not be truly representative of 'reference conditions' owing to difficulties in identifying 'unpolluted' sites in lowland regions and the somewhat subjective nature of their selection. Nevertheless, within the domain of the design, the models are quite sophisticated and provide reasonable predictions of reference communities. Classification of sites is based on a species-environment model, and application can classify river quality at sites that lie outside the bounds of the model owing to their polluted nature; although prediction at sites of markedly different character, e.g. physical dimension and conservative chemical variables such as alkalinity, from those used to develop the model are normally excluded. A developmental stage in RIVPACS was the use of EQI(ASPT) and EQI(Number of Families) for classification. The BMWP score system on which EQI(ASPT) is based was subjectively derived, and many of its scores have been shown to be erroneous (Walley & Hawkes, 1997). In addition, predictions of number of Families, and hence EQI (Number of Families), have been shown to be unreliable (Walley & Fontama, 2000, 1998a & 1998b). Thus, this crucial aspect of the system, the interpretation of the complex non-linear relationship between river quality and community structure is represented by a combination of two highly simplistic models, that are not based on relevant field data but on unreliable subjective data (i.e. BMWP scores) and unreliable predictions. The weakness of the overall system is highlighted by the fact that it classifies less than half of the 614 reference sites used to develop RIVPACS as GQA class 'a', the remainder being classified mainly as class 'b', but a few as class 'c'. This failure of the system to identify its own reference sites as top quality raises serious questions about its capability to classify polluted sites. The additional failure to utilise valuable information that can be derived from the abundance of a taxon, and also its absence, is less serious.

The basic flaw in the development of the RIVPACS-based classification system has arisen because the system as now promoted was not designed from scratch, but constructed from two existing systems, BMWP and RIVPACS. The latter had been developed for the prediction of macroinvertebrate fauna in unpolluted running waters, specifically for conservation purposes, not river quality. While incremental development of models does not necessarily undermine application, it can lead to some difficulties. In contrast the Artificial Intelligence models discussed in Chapter 4 were designed from first principles, specifically for the diagnosis of river health from biological and environmental data. They were developed using 12076 samples covering all quality classes, and are not dependent upon reference state data, BMWP scores or any other score or index. The River Pollution Diagnostic System (RPDS) simply identifies patterns in the combined biological and physical data and clusters them into 250 classes, separately for spring and autumn. Each class (or cluster) has its own unique pattern of biological, physical, chemical and stress characteristics that can be derived from the known characteristics of the sites belonging to the cluster. Thus, if a new site is classified to a particular class on the basis of its biological and physical data, its 'state of health' can be 'diagnosed' in terms of its likely stresses and water chemistry. Since diagnosis in this sense is a very fine form of classification, it provides a sound basis for the more general classification of sites into a few quality classes. However, the WFD requires that its five quality classes be defined in terms of the site's distance from its reference condition. So, for RPDS to perform such classifications it will be necessary to identify which of its 250 classes represent reference conditions. The wealth of information that RPDS provides on the characteristics of each class will do much to facilitate this task. In addition, a suitable ‘distance’ measure will have to be derived that adequately represents the non-linear nature of the relationships between the biota and river quality. One possibility is to base it on the ‘distance’ between the distributions of the actual and reference communities. This research is ongoing, but given that the AI-based systems have already proved to be valuable diagnostic and prognostic tools they clearly provide a sound foundation for the development of a robust WFD classification system. The ability to subdivide each WFD class into 50 or more sub-classes representing different types of impact should facilitate finer definition of the Good/Moderate boundary. Further discussion on the development of Bayesian modelling for predicting ecological communities is found in Ter Braak *et al.*, (2003).

Recommendations: Multimetric and multivariate classification tools require comparison and further evaluation of their application to the WFD. Like many models, they require firm understanding of the underlying principles for meaningful application.

Habitat (fish) models

In response to the need to predict impact of river regulation on fish communities a number of models have linked fish habitat preferences to river hydraulics (e.g. PHABSIM, Bovee, 1982); RHABSIM (Payne, 1994), RHYHABSIM, (Jowett, 1989), EVHA, (Ginot, 1998)). The Physical Habitat Simulation (PHABSIM) system is used by the U.K. Environment Agency to assess impact of proposed or existing abstractions on river ecology. PHABSIM contains a number of hydraulic models that predict water depth and velocity at different simulated discharges. These models require calibration using field data collected at two or more calibration discharges. Observations of substrate and cover are recorded using a coding system assumed to be independent of discharge. Once calibrated, it is claimed that the model can simulate values of micro-habitat variables over the full range of discharge within a river reach. Current research by CEH into the application of PHABSIM will be used to help to set water abstraction licences. Widespread application is, however, likely to be restricted by high data needs.

While such models can be useful in determining the response of fish to discharge and features of the habitat, and can incorporate hydraulic simulation models to predict availability of suitable habitat (Heggenes & Saltveit, 1996), they are often site specific and require precise topographical and discharge measurements. Recent work (Lamouroux *et al.*, 1999; Hatfield & Bruce, 2000; Lamouroux & Capra, 2002) has shown robust predictions of fish habitat values using hydraulic geometry and relationships between fish species and dimensionless Reynolds and Froude numbers. These models appear suitable for application across geographic scales, greater than single rivers or river sections, and for a range of species. Models applied at a river basin scale and using easily measured variables (mean width- and mean depth-discharge relationships, average bed particle size and median natural discharge) can provide reliable estimates of habitat value (Lamouroux *et al.*, 1999; Hatfield & Bruce, 2000; Lamouroux & Capra, 2002) and fish community structures. Further details of the biological preference models that relate habitat physical features of the habitat to fish communities are given in (Lamouroux *et al.*, 1998). The application of these types of models have particular importance for setting minimum flow rates (Hatfield & Bruce, 2000) and for evaluating impacts affecting discharge rates and stream-bed sediment characteristics. In heavily modified waters these models can be particularly useful in setting management objectives for both general conditions and predicting, and moderating, impacts on target threatened or rare species (Labonne *et al.*, 2003).

Further developments in using models to understand and predict fish-habitat interactions has included the use of artificial neural networks (Olden & Jackson, 2001). The authors demonstrated that species presence and absence is highly predictable based on whole lake measures of habitat, and were applicable across lakes within adjacent drainage basins. The partitioning of predictive strength into sensitivity (ability to predict species presence) and specificity (ability to predict species absence) enhanced assessment of model application. The authors claim that these models provide greater predictive power than use of traditional regressions. Artificial neural networks are discussed more fully in Chapter 4.

In Ireland, variation of fish communities will be affected more by local, rather than large-scale, biogeographic effects. The reference state for most rivers, and possibly lakes, is likely to be a fish community dominated by salmonids. The Central Fisheries Board has a well developed monitoring scheme for fish. To date, application of mathematical models in the management of inland Irish fisheries is low.

In 2002, however, under the Tourism & Recreational Angling Measure (TRAM), the CFB in collaboration with the Regional Fisheries Boards conducted a project to improve the information base on the amount and quality of freshwater habitat in Ireland. *Inter alia*, the purpose of the project was to assist determination of river specific conservation limits. The study had 3 main objectives:

- To measure the quantity of potential salmon producing habitat (wetted river and lake surface area) on a national, fisheries district and individual river system basis.

- To determine and to measure the Quality/Structure (Gradient) of potential salmon producing habitat (wetted river and lake surface area) on a national, fisheries district and individual river system basis; and

- To determine the extent of salmon 'anadromy'. The extent of 'anadromy' is a measure of the area of rivers and lakes in a catchment that can be effectively accessed by salmon entering that catchment from the sea and that is therefore available for spawning and consequently can be utilised for the production of juvenile fish.

The project developed a complex and comprehensive GIS wherein, inter alia: 261 discrete migratory salmonid 'Fishery Systems' were identified; the river width and wetted surface area within all fishery system channels was estimated based on a statistical model derived from measured width at 275 sample reaches under DWF conditions; and the extent of anadromy was estimated by linear network modelling within each fishery system, terminating at known barriers to anadromy or first order streams - the amount of habitat (fluvial and lacustrine) within each fishery system was determined - the amount of fluvial habitat with compromised water quality and potentially limiting to salmonid production (EPA 'Q value' score of 3 or less) was determined.

Recommendations: Focused models relating fish communities to impacts have a high potential for application in Ireland. Recent work on effect of salmonid streams and its link to GIS provide a firm foundation for such developments.

Ecosystem models

In general, the application of ecological models to guide management is not widespread. Models that describe or predict ecological response of single biotic "compartments" such as phytoplankton or invertebrates, to driving variables, such as nutrients, have had some success because they are conceptually simple and are often site-specific (e.g. Elliott *et al*., 2001*)*. Application of such models are only possible where moderation of biotic response to driving variables such as nutrients and flow regime are not significantly impacted upon by control mechanisms outside the immediate load-response effect of the target groups. While this situation appears to operate in rivers, and permits the long-established use of river macroinvertebrates as indicators of chemical state (Hellawell, 1986), this may be the exception rather than the norm. It may be more usual that the protential for presence of either specific organisms or functional groups is the consequence of physical and chemical conditions, which are then tempered by abiotic and biotic interactions. Generally, ecosystem structure is complex, of which the target or indicator group is merely one component.

While the emergent properties of ecological communities suggest self-organising capacity (Straskraba, 2001), such structure is also not static. Species compliments are the manifestation of a nested, or fractual series, of biotic reponse that range from intracellular to behavioural (Reynolds, 2002). Responses are frequenty non-linear (McCauley *et al.*, 1989). Strong feedback mechanisms operating within ecological systems provides a major challenge to effective, and certainly general, modelling. The non-linearity of individual species functional response, behavioural choice such as switching among prey types (e.g. Lawton *et al*., 1974), and differing response of alternate trophic groupings, illustrated by trophic cascade theory (e.g. Carpenter *et al.*, 1985; Power, 1992) provide classic examples of variable ecological response. Nevertheless, ecologist have attempted to meet these challenges and the endeavour to distil ecological communitity strucures and interactions to robust descriptive or predictive models has a rich history (e.g. Steele, 1962; Levins, 1966; Patten, 1968; Sykes, 1973; May, 1974; Maynard-Smith, 1974; Lawton, 1999). This has led to development of mechanistic frameworks of nutrient –food chain models in aquatic systems. See Chapra (1997) and Reckhow & Chapra (1999) for reviews.

With the possible exception of the application of mathematical models (Hilborn & Walters, 1992) that guide international and E.U. Common Fisheries Policy, which in any case can viewed as a special case because the modelling is not so much an integrated ecological framework rather than a species by species response to growth and harvest, mathematical modelling of biotic elements is not commonly used in the management of natural aquatic systems, and probably not at all in Ireland. Indeed, in general, the use of models developed for inland or transitional waters have been far less prevalent than hydrological and chemical ones (Westervelt, 2001). On one hand this may reflect, historically, the lack of policy-driven need but also the inherent complexity of ecosystems and the problems that poses for reliable, or broadly accepted, ecosystem models.

The need for models that can be useful for management of ecological communities and ecosystems, has driven recent important developments. Håkanson *et al.* (2003) describe a mass-balance model for phosphorus in lakes accounting for biouptake and retention in biota. Using a well developed conceptual model, driven by a low number of map (Catchment area, lake area, lake mean and maximum depth, latitude and altitude), climatic (annual precipitation) and water chemistry (pH, colour, phosphorus load) variables and using empirically derived nutrient flux estimates among six (surface water, deep water, areas of, respectively, accumulating and eroding sediments, biota with, respectively, short and long turnover times) lake compartments , excellent predictions of seasonal in-lake TP were obtained. The model provides a developement of the mass-balance approach, with a structure that can quantify abiotic/biotic feedback and which can be run on short (e.g. weekly-monthly) time-intervals. It, thereby, permits a simulation of lake dynamics responsive to changes in catchment inputs of nutrients. This is a sub-model of the larger *Lakeweb* model (Håkanson & Boulion, 2002).

Another modelling system used increasingly in recent years is the ECOPATH steady-state ecosystems model. Originally developed for coral reef fisheries (Polovina, 1984), it has been applied to a range of lakes and transitional waters (Christensen & Pauly, 1993). The model provide a mass balance among flows of energy and matter through the ecosystem, incorporating measurements or estimates of standing biomass, consumption, production, respiration and predation, parameterised with e.g. application of tropic efficiencies. ECOPATH has been developed (Pauly *et al.*, 2000) to incorporate three components: ECOPATH – a static, mass-balanced snapshot of the system; ECOSIM – a time dynamic simulation module for policy exploration; and ECOSPACE – a spatial and temporal dynamic module primarily designed for exploring impact and placement of protected areas. The model has not had widespread application in Ireland, although some preliminary systems analysis has been used to help understand the trophic exchanges within Dublin Bay (Wilson & Parkes, 1998).

Other State of the Art developments are in the field of Artificial Intelligence (A. I.) The AI-based models described in Chapter 4 were pioneered, from first principles, by Walley (an AI-specialist) and Hawkes (an experienced limnologist) in the early 1990s with a view to creating an ecological data interpretation system that would overcome the perceived weaknesses in existing systems. They believed that the data contained far more information than was been extracted by such systems, and identified several important characteristics of the interpretation process that were not being addressed by existing systems. Their approach was to model two complementary mental processes used by experts, namely plausible reasoning (i.e. reasoning under conditions of uncertainty) and pattern recognition. AI-based models developed by a team at Staffordshire University, use Bayesian Belief Networks (BBN) for plausible reasoning and an information theoretic clustering and visualisation technique (called MIR-max) that was developed by the team for pattern recognition. Under contract to the U.K. Environment Agency (R&D Project E1-056) (Walley *et al.*, 2002) these techniques were used to develop two operational systems, River Pollution Bayesian Belief Network (RPBBN) and River Pollution Diagnostic System (RPDS), which were delivered to the Agency in 2002. The integration of RPDS and RPBBN into one system with enhanced WFD functionality is now the subject of a further Environment Agency project. It is envisaged that the advanced diagnostic and prognostic features of this system will be of particular benefit in preparing '*Programmes of Measures'*.

Ecological stability of lakes depend on the strength of internal buffering mechanisms, and the importance of such mechanisms may be more pronounced in shallow than deep lakes (Scheffer *et al.*, 1993). Mathematical models that describe the relationships between nutrient loading and biotic response are seldom linear (McCauley *et al.*, 1989) and the relative response, or dominance, between phytoplankton and plant growth may vary across similar nutrient concentrations. Ecosystems may "flip" from the dominance of one state to another and may exist in mutliple stable states (Noy-Meir, 1975; May, 1977). The rate that such processes occur may be very different for the reponse of, particularly shallow, lakes to increasing (resistence to change) of decreasing (resilience to change) nutrient supply. The mathematics of these buffering systems in shallow lakes are decribed by Scheffer (1998) and, for lakes in general, by Andersen (1997). The mechanisms decribed by both authors revolve around Monod models of phytoplankton growth and nutrient uptake and stability isoclines across a number of model domains involving physico-chemisty, phytoplankton, herbivores, macrophytes and fish**.** These models have not yet been applied generally for the management of freshwaters, and remain largely of theoretical interest. However, they are gaining interest in application to specific sites (e.g. Zhang *et al.*, 2003).

Early developments in the recognition of the usefulness of alternative state modelling is the Netherlands National Institute for Public Health and the Environment (RIVM) process modelling program, PC Lake, that simulates response of biotic elements in shallow lakes to changes in nutrient loads. The model addresses water and sediment chemistry, algal and macrophtye growth and fish. Originally designed as a tool to assess critical nutrient loads to the hypertrophic Loosdrecht Lakes (Janse *et al.,* 1992), it has since been successfully applied to a number of other Dutch lakes (Janse *et al*., 1993). The model incorporates a hysteresis effect that simulates non-linear ecological switching from clear to turbid water and visa versa. More recently Aldenberg *et al.,* (1995) the model has been tested across a series of lakes using Bayesian techniques to test its statistical ability to identify patterns.

Recommendations: Models that examine non-linear response and complex dynamics within aquatic ecosystems require further research and development. They provide powerful conceptual tools for understanding structure and function of ecosystems so, while not of immediate application for the WFD, provide important clues to the relationship between State and Impact of the ecology of surface waters.

Integrated modelling of the combined pressures of eutrophication and contamination of organic toxins

Many freshwater systems are under combined pressures of increased nutrient inputs and contaminant loading from adjacent urban and agricultural sources. The interactions between eutrophication and contamination are highly complex and involve mechanisms such as: biomass and growth dilution of contaminants (e.g. hydrophobic organic compounds) in organic matter; increased sedimentation of organic-bound contaminants and uptake of contaminants in the food chain. Koelmans *et al*. (2001) reviewed integrative models that are capable of simulating chemical fate/effect and food chain accumulation at varying trophic levels and categorised them as EUTOX models. The pioneer EUTOX models are: CATS-5 (*C*ontaminant in *A*quatic and *T*errestrial eco*S*ystems) by Janse and Traas (1996); AQUATOX by Park *et al*. (1995); GBMBS model framework (*G*reen *B*ay *M*ass *B*alance *S*tudy) by USEPA (1989b); IFEM (*I*ntegrated *F*ates and *E*ffects *M*odels) by Bartell *et al*. (1988, 1992); the HOC bioaccumulation model by Ashley (1998) and an adapted version of QWASI (*Q*uantitative *W*ater, *A*ir, *S*ediment *I*nteractions) by Mackay *et al*. (1983) and Wania (1997). Koelmans *et al.* (2001) classified AQUATOX as, currently, the most complete of the EUTOX models.

The necessary linkage in EUTOX models of single issue (sub-) models dealing with: eutrophication; contamination; food web and food chain activities resulted in highly complex model types. The complexity is necessary for the inclusion of complex interactive processes between eutrophication and contamination, but carries the risk of over parameterisation and causes difficulties in calibration and validation. Principal limitations in food web modelling are the restricting factor when superimposing chemical fate model descriptions on the ecological model construct (Koelmans *et al*., 2001). Therefore, long term simulations of exposure, food chain bioaccumulation and toxicity remain uncertain on the ecosystem level. Koelmans *et al.* (2001) recommended that dominant processes should be identified, described and estimated rather than incorporation of more detail.

Despite their limitations, EUTOX models are an important development for risk assessment of aquatic systems that are impacted by combined pressures of eutrophication and contamination. The alternation of only single pressures (e.g. reduction of nutrient load) may have fundamental consequences to the ecosystem (e.g. increased bioavailability of contaminant in water column). Integrative models can simulate the interactive scenario of eutrophication and contamination that can support the environmental decision making process.

River Habitat survey

While not strictly speaking a mathematical modelling technique, the River Habitat Survey developed by the Environment Agency for England and Wales, is used widely in the UK. It provides a systematic framework for the collection and analysis of data on the physical structure of river channels and for assessing habitat quality (Raven *et al.* 1997; Fox *et al*. 1998). It has been applied across the UK and over 5000 sites exist within the Environmental Agency reference site database (Raven *et al.* 2000).

RHS was developed in response to the need for a nationally applicable classification of rivers based on their habitat quality. Four related outputs were envisaged:

- a standard field survey method (Fox *et al*. 1998);
- computer database of national reference network of UK sites;
- a classification of river types based on a predictive model of physical structure; and
- a scheme for assessing habitat quality.

The standard survey covers a 500 m length of river corridor, 100 m wide. Within this stretch, 10 spot checks and a 'sweep-up' survey are conducted. The full set of features recorded is summarised in Table 3.3. The data can be used to derive the Habitat Quality Assessment (HQA) score, which provides an assessment of habitat features that are considered important in conservation terms, regardless of river type and naturalness (Raven *et al*. 1998). Of direct significance in the assessment of hydromorphological condition is the Habitat Modification Score (HMS), which reflects the degree to which the natural stream channel and its banks have been altered (Table 3.4.). Through the calculation of the HMS it is possible to classify a river site into six classes. Where no modification is found, the site is considered unimpacted (Table 3.5.).

Two new indices are under development to assess the overall quality of the site under investigation. The first is the 'Benchmark Distance Score (BCD), which is calculated only for pristine and semi-natural sites. This index measures the departure of the HQA scores of the site and the HQA score of the nearest benchmark site (a network of reference sites equating to high ecological status). The BCD ranges from 1 to 5, with 1 being close to the reference condition and 5 being very dissimilar. The River Habitat Quality (RHQ) score is derived from the previous three scores (HMS, HQA and BCD) and this is used to assign the site into one of five quality classes (I: excellent – V: very poor). The calculation of RHQ however requires the use of the UK national RHS database – thus its application to Ireland or any new country will require an appropriate database to be developed (Buffagni and Erba, 2002).

The Environment Agency for England and Wales is continuing to develop the RHS approach through the addition of further hydrological and biotope approaches (cf. Newson and Newson, 2000); geomorphological approaches (Sear *et al.* 2002) and by further refining the determination of habitat modification to include a measure of both the degree of alteration and its longevity within the system (M. Naura, *pers com).*

Table 3.3. Summary of RHS survey data (after Fox *et al*. 1998)

Background and map-derived data	**Field survey**	
	Spot check	**Sweep-up**
General information	***Channel data***	***Channel data***
Date of survey River name Catchment name OS six-figure grid reference Altitude Valley slope Solid geology code Drift geology code Mean annual flow Distance from source Height of source Site planform	Predominant substrate: bedrock / boulders / cobbles / gravel or pebbles / sand / silt / clay / artificial / not visible Deposition features Vegetation types and extent Predominant flow type: free fall / chute / broken standing wave / chaotic / rippled / upwelling / smooth boundary turbulent / no perceptible flow / no flow (dry) Modifications	Braiding/side channels Shading of channel Trees: boughs overhanging channel / underwater roots / fallen trees Debris: dams / coarse woody / leafy Extent of: waterfalls / cascades / rapids / riffles / runs / boils / glides / pools / marginal deadwater Waterfalls > 5 m high Number of riffles / pools Artificial features: culverts / weirs / foot bridges / road bridges / outfalls / fords
	Bank data	***Bank data***
	Substrate Erosion and deposition features Modifications Bank face vegetation structure Banktop land use	Shape Modifications Flood embankments Extent of bankside trees Exposed bankside roots Number of point bars Extent of side bars
		Other site data
		Valley shape Adjacent land uses: broadleaved woodland / coniferous plantation / orchard / moorland or heath / scrub/ tall herb or rank vegetation / rough pasture / improved or semi-improved grassland / tilled land / wetland / open water / suburban or urban development Site dimensions: bank-top height and width / water width and depth / embankment heights Special floodplain features: artificial or natural open water . water meadow / fen / bog/ carr / marsh / flush Notable nuisance species: Giant hogweed / Himalayan balsam / Japanese knotweed

Table 3.4. Rules for derivation of the Habitat Modification Score (HMS) from RHS data.

Modifications at spot-checks	**Score per spot-check**
Reinforcement to banks	2
Reinforcement to bed	2
Resectioned bank or bed	1
Two-stage bank modification	1
Embankment	1
Culvert	8
Dam, weir, ford	2
Bank poached by livestock	< 3 spot-checks: 1 3–5 spot-checks: 1 ≥ 6 spot-checks: 2

Modification present but not recorded at spot-checks	One bank (or channel)	Both banks
Artificial bed material	1	-
Reinforced whole bank	2	3
Reinforced top or bottom of bank	1	2
Resectioned bank	1	2
Embankment	1	1
Set-back embankment	1	1
Two-stage channel	1	3
Weed-cutting	1	-
Bank-mowing	1	1
Culvert	8 for each	-
Dam, weir, ford	2 for each	-

Scores for features in site as a whole	One	Two or more	Site
Footbridge	0	0	
Roadbridge	1	2	
Enhancements such as groynes	1	2	
Site partly affected by flow control			1
Site extensively* affected by flow control			2
Partly realigned channel**			5
Extensively* or wholly realigned channel**			10

* Extensively means at least one-third of channel length; ** Information from map.

Table 3.5. Habitat Modification Score (HMS) Categories

HMS Score	Class	Descriptive category of channel
0 – 2	1	Pristine to Semi-natural
3 – 8	2	Predominantly unmodified
9 – 20	3	Obviously modified
21 – 44	4	Significantly modified
45 +	5	Severely modified

Introduced species

Quantitative models to predict impact of invasive species are generally lacking, but invasion history of an introduced species may provide a model for impact into a new site or region. Ricciardi (2003) used a simple regression model to predict impact of the introduced zebra mussel (*Dreissena polymorpha*) on native unionid mussels in North American lakes. In addition to the zebra mussel, a number of introduced species to Ireland will impact upon ecological status of surface waters. Examples are: the impacts of a fungal parasite, *Aphanomyces astaci*, introduced with the American Signal crayfish, on native stocks of the Irish crayfish *Austropotamobius pallipes* (Reynolds, 1988); effects of the amphipods *Gammarus pulex* and *G. tigrinus* on native gammarids (Costello, 1992) and the likely general effect on food webs by the roach (*Rutilus rutilus*). The impact of introductions on ecological reference conditions is, however, very difficult to evaluate as many species have been introduced over the last 1000 years and are now effectively *naturalised* within Irish aquatic communities. In the twelfth century the writer Giraldus Cambrensis considered that all Irish fish could live in salt water. At least seven species of freshwater fish have been introduced in the last 400 years and some may have been introduced earlier (Reynolds, 1998). A number of wetland plants are also non-native, of which the most widespread truly aquatic species is probably *Elodea canadensis.*

Recommendations: Mathematical models applicable to introduced species are not developed in Ireland and for many established species are of questionable relevance. For more recent and aggressive introductions, there is a clear need to develop mathematical models that can help predict increased range, abundance and management options.

Palaeolimnology

The WFD has a need for the definition of reference biological communities in surface waters, and the extent that departure from reference state (high status) relates to measures of *ecological quality ratios*. This is hindered through uncertainty of the extent that current conditions may deviate from reference. A means to address the general shortfall in archive information with which to judge anthropogenic driven change is through investigation of the historical record preserved in the sediment of, mainly, lakes. The science of palaeolimnology is well-established in North America and many European and countries. Palaeolimnological information collected previously in Ireland is currently being collated by the EPA funded INSIGHT project, with also a programme to collect more sediment cores in order to establish links between catchment activities and ecological status deduced from the sediment record (Smol, 2002). Mathemathical modelling is an essential part of this process.

In the sediment record, diatoms, which are sensitive to lake pH, nutrients and habitat structure, are likely to be of most general use, but may not be suitable for all lakes. Phytoplankton pigments can reflect changes in land-use practises and nutrient status and phytoplankton community composition (e.g. Gorham, 1960; Griffiths, 1978; Züllig, 1981; Foy,, 1987; Hall *et al.*, 1999; Linnane & Murray, 2000). Changes in lake ecology can also be deduced from the sediment remains of a number of other biotic groups. These include: cladocerans (D.G., 1960; Goulden, 1966; Parise & Ravera, 1982; Jeppesen *et al.*, 2002); chironomids (Walker, 1995), pollen (Edwards & Whittington, 2001; Huang, 2002) and the macro-remains of plants. Changes in a sediment core in P, Fe, Mn, Ca, Na and K can be used to provide information on the degree of catchment disturbance (Rippey & Anderson, 1996).

Robust relationships of diatoms with pH (Battarbee, 1984; Jones *et al.*, 1986; Anderson & Korsman, 1990) and P (Hall & Smol, 1992; Bennion *et al.*, 1996) have been developed using diatom indices, multivariate statistics and the transfer function approach. This requires establishment of *training sets* for the quantification of relationships between diatom abundances in surface sediments and pH and TP, using correspondence analysis (e.g., DCA and CCA), and the development of diatom transfer functions (TFs) for TP and pH using, e.g., weighted averaging techniques (Hall & Smol, 1992). Modelled relationships can be applied throughout the sediment core and include a number of other relationships with biota, using a multi-proxy approach. This allows a number of elements to be used and cross-validated (e.g Brooks *et al.*, 2001; Jeppesen *et al.* (2001) and application of a variety of groups when e.g preservation of diatoms may be poor. Cores can be dated through a variety of, usually, radiometric techniques.

Recommendations: Reconstruction of historical conditions using modelled relationship and transfer functions is a potentially powerful tool to assist with the determination of reference conditions and assessment of anthropogenically induced change. These techniques should be applied across lakes for which there is, and has been, palaeolimnological study

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3.4.4. Transitional waters

In contrast to hydrological and water quality model, ecological models in transitional waters are still largely in a developmental stage. With similarities to ecological models developed for lakes and rivers, this reflects the added complexity and uncertainty inherent in the predictability of ecological, and particularly community, processes. Ecological models that have been applied to transitional waters can be broadly grouped into the general and the specific. General models include those which model a variety of ecological processes, including growth, and productivity and/or biogeochemical processes which drive or which influence the ecology. Examples of general ecological models would be the ICES fisheries models:
(http://www.ices.dk/datacentre/software.asp) in which a restricted range of parameters are required for a strictly controlled output. The basic fishery model is based on a single species Virtual population Analysis (VPA), in which the required input data are age/size/growth, with an output forecast of population size (numbers and biomass including harvestable biomass) for a specified time in the future. While they are not system models, they can be used with some certainty for selected compartments, and they have the benefit of a great deal of testing and development behind them. They are also being developed in to more reliable multi-species models, into which biological processes such as competition and predation may be incorporated, as well as environmental variables such as water temperature or salinity.

To date, very few specific ecological system models have been constructed and run successfully. Those that have been, tend to be fitted to a certain situation such as large scale modelling efforts in Chesapeake Bay (Kemp *et al.*, 1995) and its catchment (Carpenter *et al.*, 1985) the North Sea (ECOHAM, ERSEM), and strictly outside the domain of transitional waters. However, ERSEM has been extended into a generic model that describes the pelagic and benthic ecosystems and the coupling between them. This model was developed during the European MAST project ERSEM I 1990 – 1993 (described in a special issue (Number 33) of the Netherlands Journal of Sea Reserach)., Lenhart *et al*. (1995). Structural refinement and several applications were realized in the project ERSEM II 1993 – 1996 (see special issue of the Journal of Sea Research 38(3-4)); Baratta-Becker *et al*. (1997) and Ebenhoh *et al.* (1997).

The Long Term Trend (LTT) Application focussed on the eutrophication of the North Sea in the second half of the twentieth century. However, this model has not yet been rigorously tested in estuarine conditions, but it is available to be downloaded at http://www.ifm.uni-hamburg.de/~wwwem/dow/ERSEM/

More specialised are the ECOPATH models and the STELLA type system models, in which the models are fitted to processes or transfers to give a mathematical framework through which the chains or networks can be modelled. These models are attractive because they can be used to provide scenario assessments to changing pressures or management, but are susceptible to bias through insufficient data or inappropriate conceptual model linkages. As discussed in section 3.4.3, *'Ecosystem Models'*, ECOPATH has been applied to help understand energy flows through a range of coastal fisheries.

General geochemical models are more common, (see e.g. LOICZ/IGBP node) and have reached a high level of integration into hydrodynamic modelling. They can also be used to drive some of the ecological models through the generation of the input or boundary data.

The geochemical models vary greatly in the degree of simplification. "Budget models" are simple mass balance calculations of specific variables (such as water, salt, sediment, CNP, etc.) within defined geographic areas and over defined periods. Usually budget models are built to aggregate the many small individual pieces of a system into smaller sets of pieces which are similar to one another. Thus, all plant species in an ecosystem might be aggregated into "primary producers." Some grouping will occur for almost any model. As one applies a single model across a range of systems, the value of such groupings becomes readily apparent. For some purposes it may be adequate to group all organisms within an ecosystem into the "net biogeochemical reactions" which occur within the system. The next step is from these simple, highly aggregated, models to more complicated models which describe specific processes (e.g., primary production as a function of light; sediment transport as a function of river flow, etc.). Many such process models may be further combined into an integrated system model. However, in general, the more complex the model structure, the less statistically robust is the statistical output. These complex models are generally ‘highly tuned’ for specific sites, requiring relatively large amounts of site specific measured data and they are not usually highly transportable.

LOICZ Biogeochemical Modelling Guidelines have been produced (Gordon *et al*. 1996) and may be summarised as follows:

- Construction of many local budget models, following an internally consistent budgeting procedure;
- Comparison of these budget models to seek patterns of similarity or difference in material fluxes.
- Statistical extrapolation of the fluxes to other situations

A range of models have been developed in the ECOFLAT project (http://www.nioo.knaw.nl/cemo/ECOFLAT/main.htm). These include attempts to predict the distribution and abundance of animals or chemical substances, and their change over time. ECOFLAT includes models for: microbiological processes in the sediment to estimate diagenisis of organic matter, oxygen and nutrients and algal production; water movement and transport of mud and organic matter to estimate location and rates of sedimentation; and an over-view of the importance of intertidal mudflat processes for the estuary as a whole.

Also freely available is NTWRK, and while this is an analysis routine rather than a modelling routine *per* se, it can be adapted as such by fitting the systems (adjusted and completed where necessary by AUTOMOD and DATBAL) to STELLA or ECOPATH models. This has a number of advantages, not least that it requires much less data, notably for the processes, much of the needed data is currently available, and the network analysis itself generates a series of metrics by which the performance of the system can be quantified and measured. However, it should be re-emphasised that this is not at the stage of predictive modelling

ERSEM and ECOFLAT are being developed by a team led by NIOO-KNAW in the Netherlands, but the models have not yet been tested at system level elsewhere. However, the process models on which they are largely based have in the most part been widely used and can be incorporated with confidence into any selected framework. There is potential for incorporation into the WFD implementation in the median – long term.

Vollenweider-type models may be appropriate for estuarine situations, although some of the difficulties of applying these models (discussed in section 3.4.3, '*Modelling the chlorophyll-TP response in lakes'*) can be accentuated under the more complex physical dynamics found in transitional waters. Nevertheless, Smith, *et al.*, (1999) considered that critical nutrient load (Vollenweider-type) models could be useful for defining:

- relationships between spring or summer concentrations of chlorophyll and late winter maximum concentrations of dissolved N;
- the critical load, or concentration of N that yields a critical concentration of chlorophyll; and
- the degree to which current loadings exceed critical loads.

Application of a critical load approach for management of nutrient loads has been reported for to a number of estuarine and coastal waters (e.g. (Vollenweider *et al.*, 1992; Wallin *et al.*, 1992; Hessen *et al*., 1997; Wallin & Hakanson, Persson, J)

Recommendations: The most commonly used modelling systems internationally for shallow transitional waters are the two-dimensional depth-integrated models. Typically these models are modular in form consisting of hydrodynamic, solute transport, sediment transport and water quality modules. Models generally have horizontal grid resolutions of between 30-150m and can be run on standard PC's. A recent DIVAST model developed of the Mersey Estuary for they UK Environment Agency simulates all hydrodynamics and 13 water quality parameters at a 100m grid spacing. The model runs on PC and can simulate 30days in approximately 17hours. This model has a sophisticated GIS interface developed using ArcView with on-line help which allows Agency staff perform in-house simulations.

Such models are now considered fundamental to process modelling of transitional waters and they allow users to simulate nutrients, oxygen, phytoplankton, diatoms and metals. The UK Environment Agency and other national agencies are currently using these types of models for analysing and managing major estuaries. In implementing the Water Framework Directive in Ireland it will be necessary to apply such models to relevant transitional water bodies. Following the approach of the UK Environment Agency, ideally a library of models of transitional waters should be developed in standard format and maintained by a central agency. The models should have user-friendly interfaces so that they can be used subsequent to the end of particular modelling projects. The results form water quality models may used directly or indirectly to assess ecological status or the models may be linked to other ecological models such as ECOFLAT.

3.4.5. Total Maximum Daily Loads (TMDLs)

A programme to establish Total Maximum Daily Load (TMDL), the maximum amount of a pollutant that a waterbody can receive and still meet water quality standards, is required by section 303 (d) of the US 1972 Clean Water Act. TMDLs are required for all waters that do not meet water quality standards, even after point sources of pollution have installed the minimum required levels of pollution control technology. They are also used as a management tool to maintain quality standards. The principle of TDMLs is that they represent an *assimilative* capacity (Havens & Schelske, 2001) of the receiving waters with respect to the specific pollutants or pollutants and which is compatible with designated use for e.g drinking water, fishing and recreation. Following many years without implementation of TMDLs, legal action by citizen organisations has encouraged the US EPA to establish TMDLs and there is now a programme to effect this
(see http://www.epa.gov/OWOW/tmdl/case.html for some case studies).
In proposing or listing waters, either impaired or threatened by pollutants, States, territories, and authorized tribes must consider "all existing and readily available water quality-related information", including for each waterbody, the pollutant(s) that is(are) causing the impairment. TMDLs are set with public consultation, and while not explicitly following an Ecological Quality Ratio approach relative to Reference Conditions required by the WFD, in practice estimations of reference conditions are often relevant in setting targets e.g. Heiskary (1989), and certainly for reporting overall regional water quality status (EPA, 1998). In the US, it is common that “reference sites” are identified as either the upper 75% of “high quality” sites, or the upper 25% of all sites. This statistical approach based in frequency data is not the same as the concept of reference state defined in the WFD. Nevertheless, the TMDL approach has many similarities to the policies of the WFD. For overview of the US approach also see http://www.epa.gov/owow/tmdl/overviewfs.html.

The USEPA (USEPA, 1999; USEPA, 1999; USEPA, 2001) has developed protocols for developing TMDLs in response to a number of pollutants. TMDLs are site specific and must include the total of all point and diffuse loads and incorporate a margin of error. They must also take into account seasonal and spatial variability of load and impact, and in its development characterise the catchment to identify all sources of pollutants as well as background loads. A TMDL implementation plan is analogous to the WFD *Programmes of Measures.* It requires measurable indicators, in appropriate units, and target values to evaluate attainment of water quality standards; and monitoring and use of modelling to determine effectiveness of control measures. Qualitative assessment of waters is allowed where quantitative measures are not available or appropriate, such as for some biotic variables.

Mathematical modelling is employed frequently in the setting of TMDLs. For example, for Wolfe Lake, Mississippi, the TMDL requirement involved estimates of land-use specific loads using the *Generalised Watershed Loading Function* (GWLF) model (Haith & Shoemaker, 1987; Haith *et al.*, 1992). This program uses literature values for runoff, sediment and groundwater relationships in different parts of the country, and estimates streamflow, nutrient loads, soil erosion and sediment yield. As Wolfe Lake has seasonal patterns of stratification, a 2-D water quality model such as CE-QUAL-W2 (Cole, & Buckak, 1995) has been used to simulate eutrophication processes and which allows evaluation of seasonal scenarios of management in relation to dissolved oxygen standards. Setting of TMDLs commonly include uncertainty analysis and include a statistical probability around the target measure. For example, to achieve a 4.5 μg l^{-1} target for chlorophyll *a* for Lake Chelen, Washington, the TMDL established a target TP load of 51 kg P day-1, and so that there was a 95% probability that the lake would remain ultra oligotrophic (USEPA, 1999).
http://www.nmenv.state.nm.us/swqb/Centerfire_Creek_Plant_Nutrient_Draft_TMDL_10-09-01.PDF provides further example of the setting TMDLs. Havens & Schelske (2001) discuss the importance of considering biological processes when setting a TMDL for phosphorus.

Simple models that have been employed to set and help implement TDMLs range across relationships of e.g lake trophic status (Carlson, 1977), generalised land-use-nutrient load regressions for urban (Tasker & Driver, 1988) areas and Vollenwider type regression models. The mid-range complex models include GWLF and AGNPS, BATHTUB, EUTROMOD and the most complex include BASINS, DRM3-QUAL, CE-QUAL-W2, HSPF, SWMM, SWAT, WASP 5, PHOSMOD (section 3.3). A decision framework for identifying modelling options relating transfer from source to water body and, onto water quality targets as recommended by the USEPA (1999) are shown in, respectively, Figures 3.10. and 3.11.

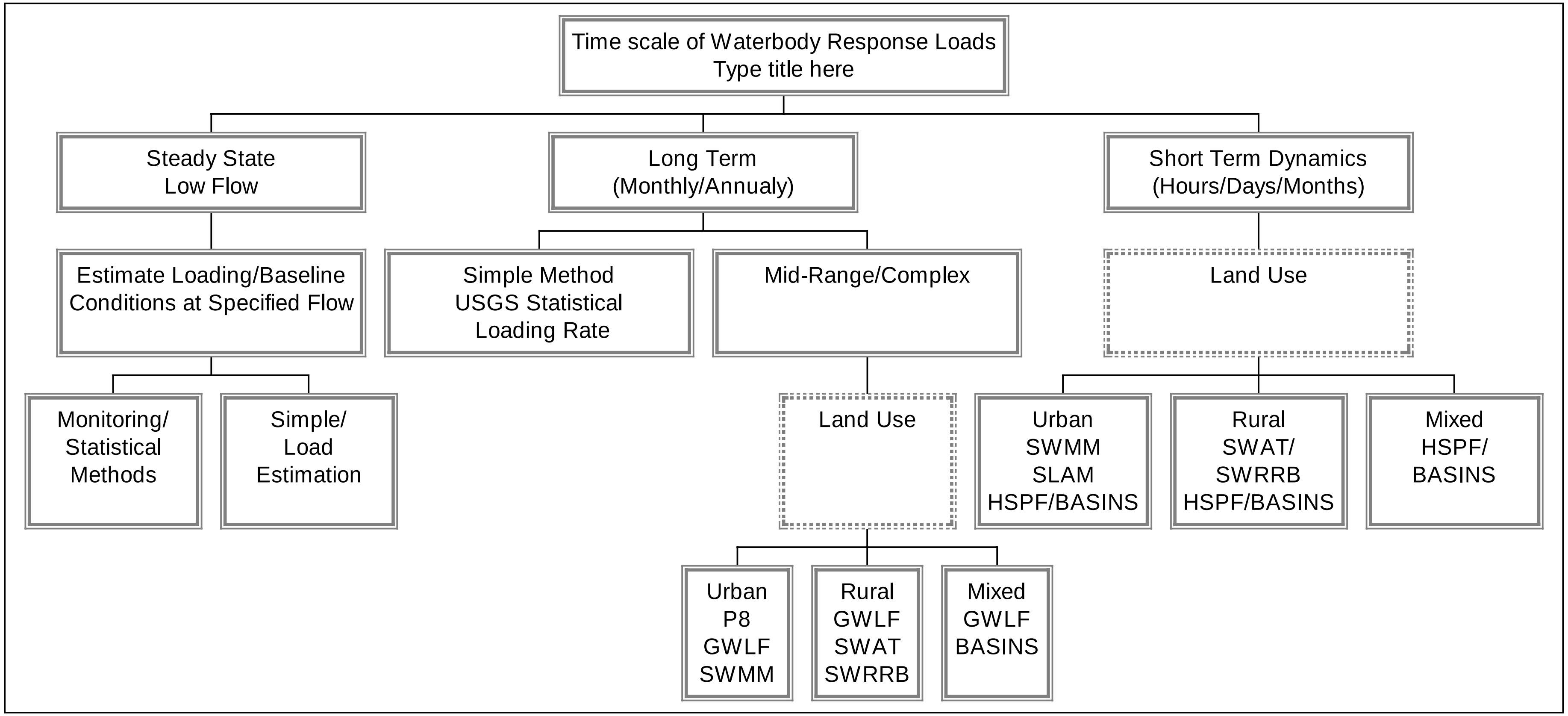

Figure 3.10. Decision tree with preferred model selection options

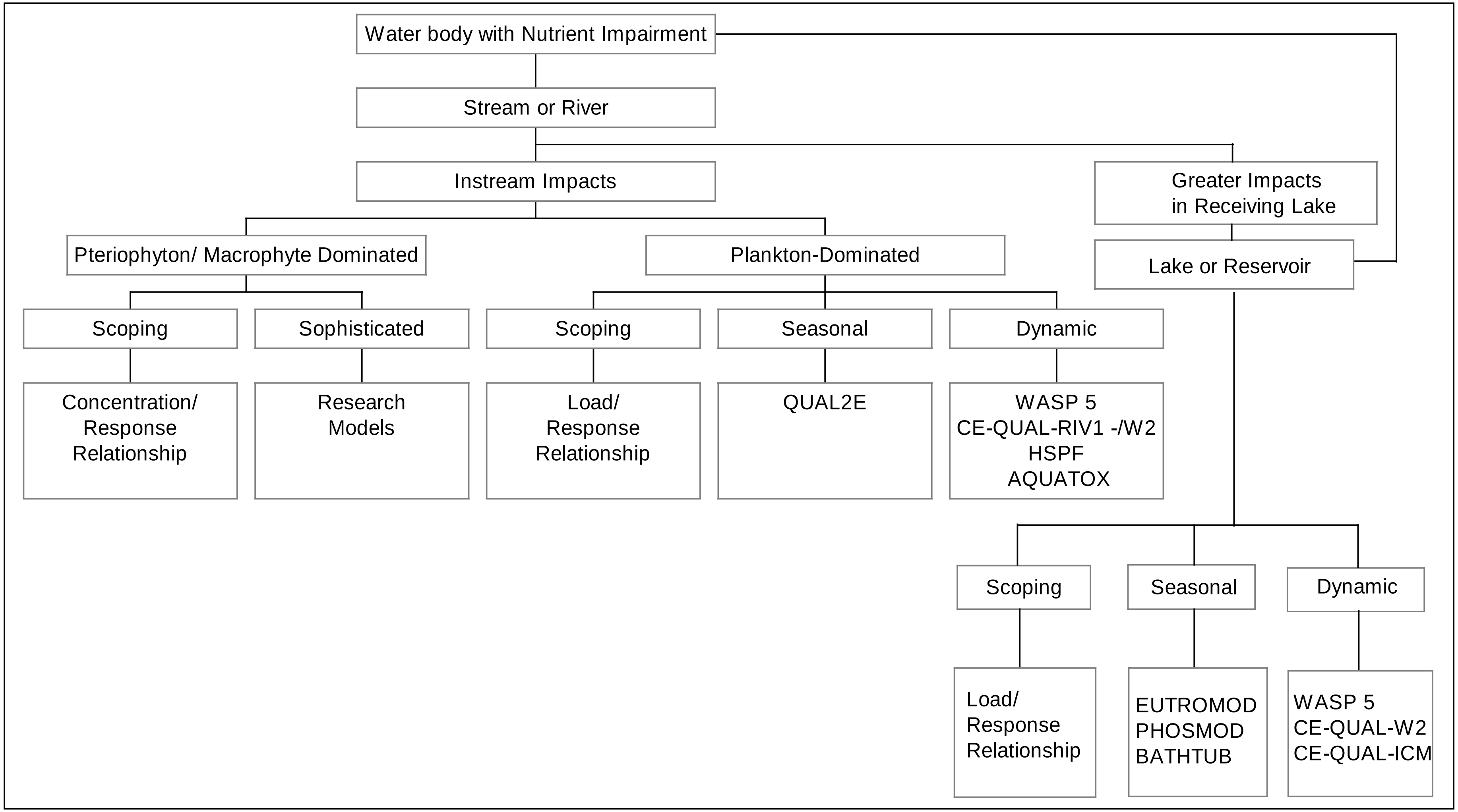

Figure 3.11. Decision tree for selecting an appropriate model technique.

CHAPTER 4 ARTIFICIAL INTELLIGENCE-BASED MODELS OF ECOLOGICAL HEALTH

4.1. Introduction

The Artificial Intelligence (AI) approach to the interpretation of biological and environmental data into river quality terms was pioneered in the early 1990s by a team at Aston University (Walley *et al*., 1992; Ruck *et al*., 1993; Walley 1994). The approach aims to simulate two complementary mental process that are used by experts when interpreting field data, namely plausible reasoning (i.e. using ones scientific knowledge of the ecological system) and pattern recognition (i.e. using ones experience of former cases to identify meaningful patterns in the data). Experts subconsciously combine these two processes to reach a final conclusion. The work pioneered at Aston University was brought to fruition by the Centre for Intelligent Environmental Systems (CIES) at Staffordshire University, under the guidance of Professor Bill Walley. A series of Environment Agency (EA) research projects resulted in the delivery of two operational models in 2002:

- River Pollution Diagnostic System (RPDS) based on pattern recognition; and
- River Pollution Bayesian Belief Network (RPBBN) based on plausible reasoning.

RPDS is the most advanced of the two models since it has been under development longer than RPBBN, which is still considered a prototype. Thus, RPDS has a comprehensive user-friendly interface that gives access to many useful diagnostic functions. In fact the software reached the finals of the British Computer Society's Technology Awards (2003). RPBBN offers both diagnostic and prognostic capabilities within a single user-friendly model, but has limited functionality. Both models are being developed further as part of a current EA project, and will eventually be integrated into one system. A prognostic capability will be added to RPDS and greater functionality added to RPBBN.

In addition to these two operational models, CIES has developed an information theoretic pattern recognition system called **MIR-max** (Mutual Information and Regression maximisation) which was used for the development of RPDS. MIR-max is a user-friendly system for the development of diagnostic or prognostic models from data.

Full details of the development and testing of MIR-max, RPDS and RPBBN were reported by Walley *et al*. (2002).

CIES also developed software called BBN Creator for the creation and implementation of Bayesian Belief Networks, but this has not yet been packaged for general use. However, commercial BBN development packages are available (e.g. HUGIN and Netica), but they require programming skills for the development and implementation of BBNs for real-world problems.

The following sections explain the basic foundations of the AI approach and then describe the development systems and operational models mentioned above. The development systems are dealt with first for the sake of clarity of understanding of the methodology.

4.2. The Basic Foundations of the AI Approach

The RPDS and RPBBN models were both based on some general principles that were established during the early stages of the development of the AI approach. Since these new methods of interpreting biological data were developed from first principles they differ from established methods, not only in their mathematical formulations, but also in their use of the data.

The AI approach starts from the premise that the way in which real experts perform their tasks provides a good foundation for the development of computer based "expert systems". In this approach, the biota act as witnesses (or sensors) of the 'state of health' of the river'. Their evidence is given in terms of their 'state of existence', which may vary from 'absent' to 'highly abundant'. Their collective evidence is interpreted using the mathematical techniques of plausible reasoning and pattern recognition. Important characteristics of the problem are considered to be:

1. inherently *uncertain* in the meaning of the evidence given by each taxon;
2. the *holistic* way in which real experts treat the biology of ‘clean’ and ‘dirty’ waters;
3. the *holistic* way in which real experts interpret field samples;
4. the *non-monotonic* nature of human reasoning (i.e. the ability to change ones mind if new evidence ‘explains away’ existing evidence);
5. the bi-directional nature of human reasoning (i.e. cause to effect / effect to cause);
6. the fact that biological and environmental data contain a large amount of hidden *information* about the river’s state of health; and
7. that the subject of the analysis is a complex non-linear *system*.

When first developing the AI approach it was concluded that:

8. the abundance of a taxon provides more evidence than just its presence; and
9. the absence of commonly occurring taxa also provides valuable evidence.

It is also well known that:

10. identification to species level is more informative than to genera or family level;
11. some taxa are much better indicators (i.e. witnesses) than others; and
12. the season and site type, in addition to water quality, are important factors governing the composition of the biological community.

Thus, the AI models (RPDS and RPBBN) were designed to:

- handle uncertainty in a mathematically sound and consistent way;
- be holistic and non-monotonic in their interpretation of data;
- reason bi-directionally (RPBBN only);
- maximise information extraction (mainly RPDS);
- conform with systems theory, and model non-linear relationships;
- use abundance data (including ‘absent’ as zero);
- include the effects of site characteristics and season;
- use biological and site type data as inputs for diagnoses;
- use chemical and site type data for prognoses (presently RPBBN only);
- automatically take account of the indicator value of each taxon; and
- minimise the subjective input to the modelling process.

4.3. MIR-max: A System for the Development of Pattern Recognition Models

MIR-max was designed for the development of ecological models for the diagnosis of river health based on pattern recognition (classification) and data visualisation (O'Connor and Walley, 2000; Walley and O'Connor, 2001). Initially its design was based on the Self-Organising Map (SOM), a standard form of unsupervised-learning neural network that performs holistic classification. However, this was later abandoned in favour of an information theoretic approach developed specifically for the purpose at CIES. There were two main reasons for the change. Firstly, the SOM algorithm does not achieve optimal clustering of the input data, because it integrates the clustering and ordering processes into one process. Since optimal clustering is vital to reliable diagnosis, the MIR-max algorithm separates the two processes and gives priority to clustering by performing it first. The resulting clusters are then ordered in output space. Secondly, the biological data supplied by EA were ordinal (i.e. abundance ratings), not interval-valued as required by SOM. The information theoretic approach does not make use of a distance measure, Euclidean or otherwise, and is ideally suited for use on ordinal data.

The Mathematical Basis of MIR-max

Hierarchical clustering techniques (e.g. TWINSPAN) do not classify the data holistically, but place greater emphasis on specific features, thus making them more vulnerable to incorrect classification. The MIR-max algorithm clusters the data holistically into n classes by maximising the mutual information between the n classes (C) and the m attributes (X) (e.g. BMWP families) of the samples. If each of the attributes X_j (j = 1 to m) can occur in one of s states (k = 1 to s, e.g. absent, rare, common, abundant), then the mutual information $M(C, X_j)$ between the classes C and attribute X_j is given by:

$$M(C, X_j) = \sum_{i=1}^{n} \sum_{k=1}^{s} \alpha_{ijk} \log_2 \left(\frac{\alpha_{ijk}}{\beta_i \gamma_{jk}} \right)$$

where: α_{ijk} = probability of finding attribute X_j in its k-th state in class C_i

β_i = prior probability of class C_i

γ_{jk} = prior probability of finding attribute X_j in its k-th state.

(Note. The prior probability is the probability of the event in question based on past experience and in the absence of any evidence to the contrary. Thus, the prior probability of class C_1 can be estimated from the database as the number of C_1 sites divided by the total number of sites.)

The overall mutual information G across all m attributes is given by:

$$G = \sum_{j=1}^{m} M(C, X_j)$$

The aim of the optimisation procedure is to maximise G.

Once the samples have been clustered into n classes, the MIR-max algorithm orders them in a two-dimensional output space such that their relative positions in data space are preserved as closely as possible. The output space has z possible locations for the n clusters, where $z \geq n$, and may be based on a triangular or rectangular grid. If $z = n$, or is marginally greater than n, the clusters are tightly packed in the output space, but if $z >> n$ they are sparsely packed. The correlation coefficient (r) between distances in data space and distances in output space is used as the measure of how well the output map represents the relative positions of the classes in data space. Thus, the aim of this optimisation procedure is to maximise r.

Full details of the optimisation procedures used to cluster and order the data are given in O'Connor and Walley (2000) and Walley and O'Connor (2001).

The User-friendly Interface

The MIR-max interface divides the development of a new model into a series of six self-contained steps that are easy to follow. These enable users to make later modifications to parts of the model without having to go through all the steps again. The user selects the step to be performed from the main menu. The six steps are outlined below.

Create/Edit an Indicator File.

The user reads in the source data, selects the indicators to be used, defines their ordinal bands, and saves the information as an *Indicators* file.

MI-max Clustering

The user defines the number of clusters to be formed, then the data are clustered using only those indicators defined in *Indicator* file. The results are automatically saved in two new files, *Clusters* and *Clustered*. The first gives the cluster ID to which each sample has been allocated, and the second summaries the characteristics of each cluster.

Create Base Map

In this step, the user selects the size and shape of the base map on which the clusters will be ordered, and this is automatically saved as a *Map* file.

R-max Ordering

The user selects the clusters (as defined by a *Clusters* file) and base map (as defined by a *Map* file) to be used in the ordering process. The results are saved in a *Mapping* file. This completes the training of the model.

Create a Configuration File

The user has to create a *Configuration* file by selecting the *Indicators, Clusters, Clustered, Map and Mapping* files that define the model. This approach to model definition allows the user to modify the model without having to repeat the whole process again.

View Clustered and Ordered Data

This final option on the main menu allows the user to view and explore the model.

Figure 4.1. shows a typical screen of a MIR-max model that was trained using invertebrate and physical data from the Republic of Ireland. On the left of the screen is an output map showing 100 clusters that have been ordered within a Hex10 (i.e. a hexagon of side length 10) base map. In this particular case, the map is displaying the probability of ‘Clean substrate’. The user can choose to display any one of the variables (or features) that were in the original data file, whether or not they were used to train the model. These maps are referred to as ‘feature maps’.

The right side of the screen is reserved for six tabbed function windows.

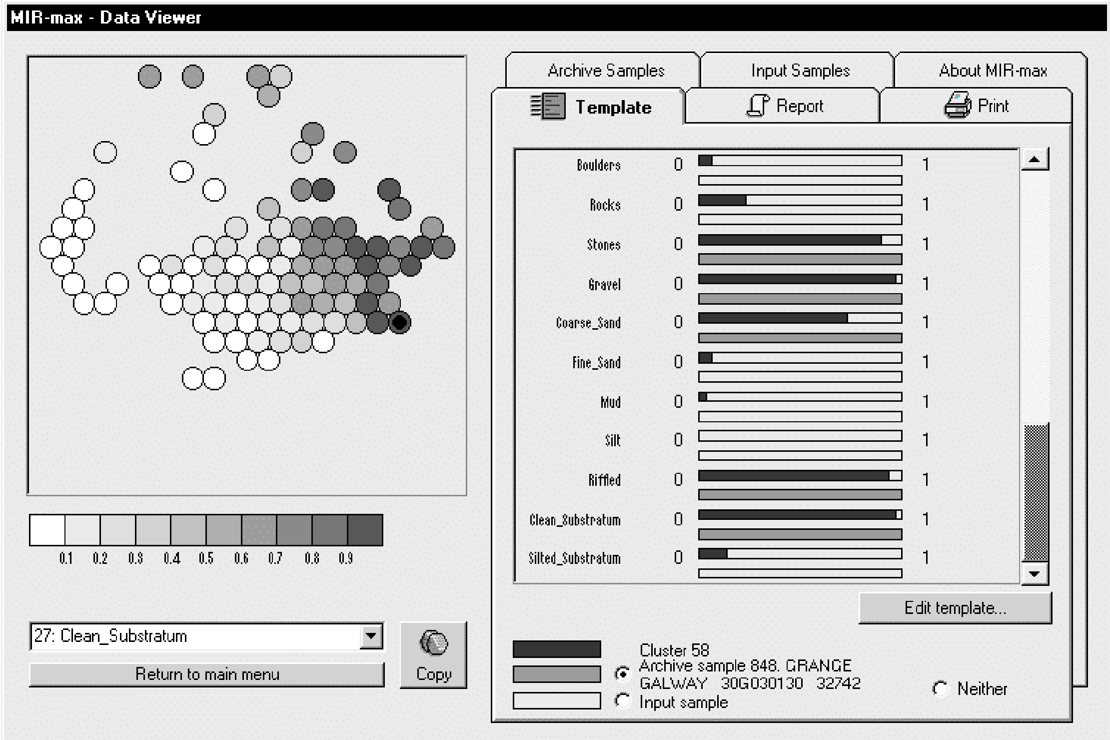

Figure 4.1. The output screen of a trained MIR-max model, showing (on the left) a typical feature map and (on the right) a typical template and the tabs of five other function screens.

- Archive samples - allows the user to select one of the samples from the original data.
- Input samples - allows the user to input and classify a new sample from file.

- Template - allows the user to design and display a template showing a histogram of the magnitudes of a selected set of variables (e.g. invertebrates, physical characteristics, chemical variables) for any chosen cluster, archive sample or new input sample. In Figure 1, only the selected cluster (indicated by a black spot in the centre of the cluster) and an archive sample from the same cluster are displayed. The template window can be scrolled, thus allowing the user to view as many variables as desired.
- Report - gives details of the characteristics of any selected cluster (i.e. the mean, minimum and maximum values of each of its input variables, plus the number of archive samples classified to the cluster and a list of the samples).
- Print - allows the user to print details of the characteristics of any selected cluster or details of any selected archive or new input sample.

- About MIR-max - provides basic details of the MIR-max system.

4.4. RPDS: An Operational 'River Pollution Diagnostic System'

Overview

RPDS was developed for the Environment Agency of England and Wales as part of National R&D Research Project E1-056 (Walley *et al.*, 2002). The core component of RPDS is a MIR-max model that was trained using data supplied by the Environment Agency and validated by CIES. The model classifies site samples (i.e. biological + environmental data sets) into one of 250 clusters arranged in a hexagonal output space. The validated data used to train the model consisted of spring and autumn records from 6038 river sites in England and Wales that were sampled in 1995. Each record consisted of the abundance levels of 76 macroinvertebrate families and 11 environmental variables. RPDS also uses data on the types of stress affecting each of the sites (e.g. effluent from sewage treatment works, pesticides) and water chemistry (up to 38 variables, depending upon availability). RPDS was written and compiled using Microsoft Visual Basic 6, and is designed for use on 32-bit Windows platforms.

Functionality and User Interface

The RPDS interface is a purpose designed extension of the interface used for MIR-max models. The main RPDS screen is shown in Figure 4.2. Its main features are described in the following subsection.

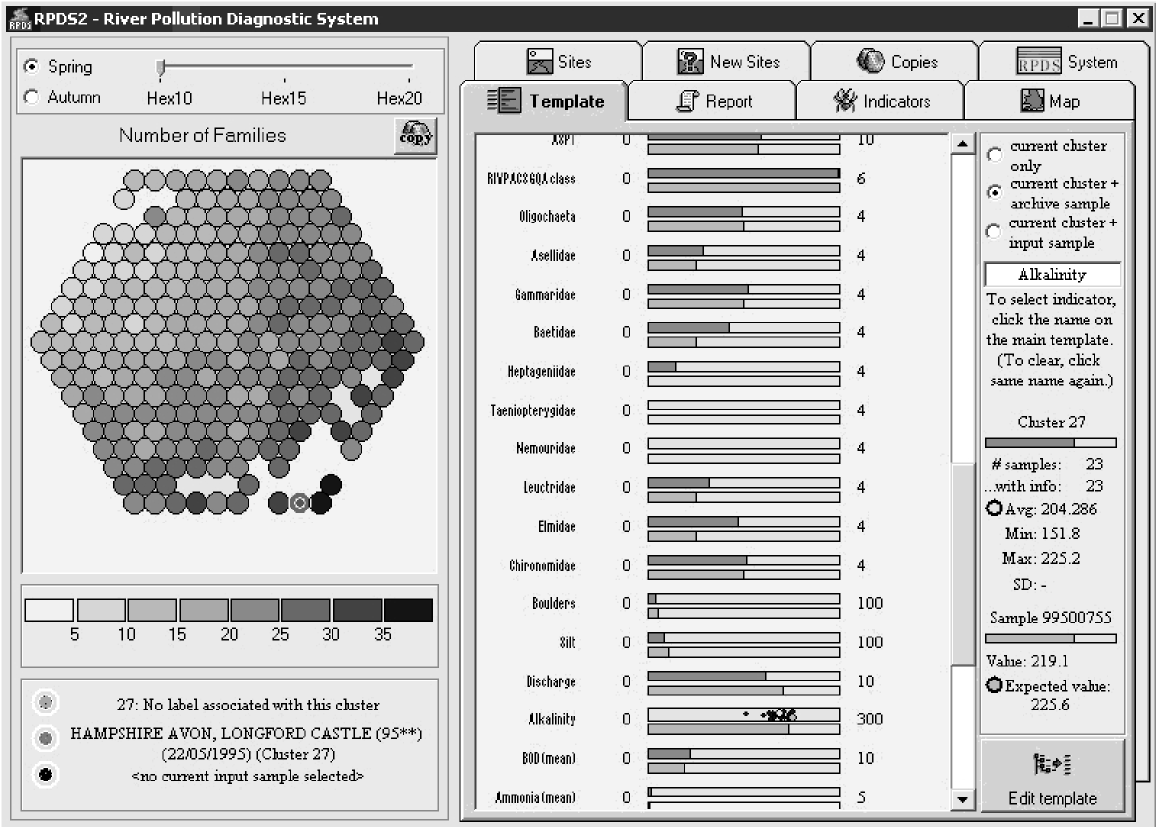

Figure 4.2. The main RPDS screen showing the model selection panel (top left), the feature map / classification panel (middle left), the status panel (bottom left), the tabbed function panels (right) with the Template panel displayed.

Model selection panel

RPDS has two basic models, spring and autumn, each with 250 clusters. These can be displayed on three different hexagonal base maps (i.e. Hex10, Hex15 and Hex20), thus allowing the user to view densely packed feature maps or more sparsely packed maps. The panel allows the user to select the model and map size.

<u>Feature map / Classification panel</u>

The Feature map / Classification panel displays the 250 clusters for the chosen model on the selected based map. When used to display a feature map of an indicator, selected via the tabbed *Indicators* panel, each cluster is represented as a coloured circle (transposed to a grey-scale here), the colour depending on the average magnitude of the indicator in that cluster. The feature map shown in Figure 2 is the average 'Number of Families' found in the samples in each cluster. It indicates that the clusters in the top left of the map represent sites having less than 10 families, whereas those on the right of the map tend to represent sites with at least 25 families.

The gradual variation in Number of Families across the map, illustrates the point that MIR-max orders the clusters so that near neighbours are similar and distant neighbours are dissimilar. Feature maps can be displayed for any of the 87 training variables (i.e. 76 BMWP families and 10 physical characteristics plus alkalinity) and/or 68 supplementary variables, including 26 perceived stresses (e.g. farming, sewage treatment works), 37 chemical variables (e.g. pH, TON, zinc) and five miscellaneous variables (e.g. Number of Families, ASPT, GQA class).

The Hex10 base map shown in Figure 4.2 has 271 locations in which to order the 250 clusters, so there are very few spare locations. This means that in some cases near neighbours may have been forced together despite being not very similar. If mapped onto a larger base map with more grid-point locations (e.g. Hex15 or Hex20 with 631 and 1137 locations respectively), such clusters are able to move apart to form a more disaggregated map. These maps provide a more accurate reflection of the relative distances between the clusters in data space, but loose some of their map-like character. These different types of map provide complementary aids to data visualisation, and hence to the user's understanding and interpretation of the problem.

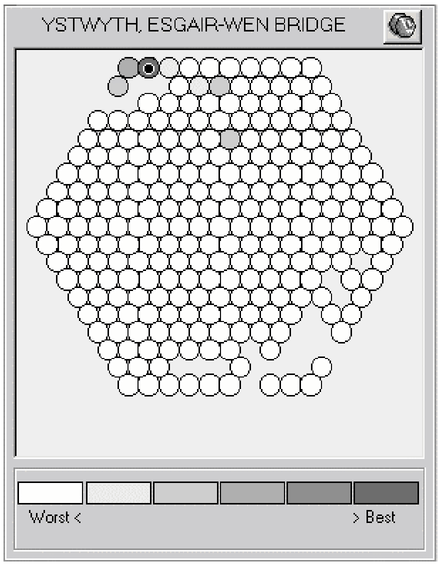

Figure 4.3. Classification of a *New site*

When the output map is used for the classification of a sample from a new site, as in Figure 4.3, it indicates the cluster to which the site has been classified by means of a green dot (in this case black) and displays the site's name above the map. The classification is based on the best 'match' between the input template of the sample (NB. In RPDS this consists of 76 BMWP and 11 environmental variables) and the corresponding template of the class exemplar. However, the best 'match' is not based upon a distance-based similarity metric, but on the degree to which the sample would increase the overall mutual information if added to the class in question.

The next best alternative classifications are indicated by a colour-coded scale (grey scale here) from 'Best' alternatives to 'Worst' alternatives. In this example, a neighbouring cluster was identified as the best alternative classification.

The feature map display panel only allows one map to be displayed, but each can be 'captured' and displayed in its own window by use of the *Copy* button (top right of the feature map panel). This enables the user to compare the feature maps of two or more variables alongside each other.

<u>Status panel</u>

This panel enables the user to keep track of the information currently being displayed by RPDS. Up to three separate clusters may be highlighted on the output map. These are: the current cluster (chosen by 'point and click' on the feature map); the cluster containing a selected *Archive sample* (chosen using the *Sites* function panel); and the cluster to which an *Input sample* (chosen using the *New Sites* function panel) has been classified.

<u>Tabbed function panels</u>

There are eight tabbed function panels: *Sites*, *New Sites*, *Copies*, *System*, *Template*, *Report*, *Indicators* and *Map*. *Sites* and *New Sites* allow the user to select an *Archive sample* (i.e. one used in the training of RPDS) or a new *Input sample* from file. *Copies* allows the selection and display of four feature maps to a reduced scale. *System* provides basic information about RPDS. *Indicators* allows users to select the variable to be displayed in the *Feature map* panel. *Map* displays the geographic location of the sites that form the current cluster, as displayed in Figure 4. In this example, the cluster represents the most acidic sites in England and Wales. The remaining two function panels are described in greater detail below.

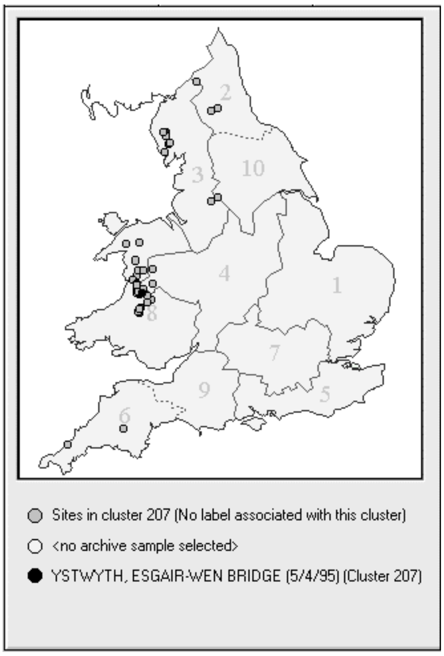

Figure 4.4. Map showing the distribution of sites in a selected cluster.

<u>Template panel</u>

Templates show the data patterns relating to a particular site or cluster. The user can select the variables to be included in the template by clicking on the 'Edit template' button. Templates can consist of any subset of the 87 training variables and 68 supplementary variables. Once designed, the template can be saved and displayed, but no bars will appear on it until the user has selected a cluster on the feature map.

The template then displays the pattern of data represented by that particular cluster. If an *Archive sample* or new *Input sample* is then selected its data pattern is displayed alongside that of the current cluster. If the sample belongs to (or has been classified to) the current cluster, then the template indicates how well the sample matches the cluster's 'exemplar pattern', as shown in Figure 2. If the sample belongs to a different cluster, the template indicates the magnitude of the mismatch between the two. When a new *Input sample* is classified to a cluster, the values of any supplementary variables on the cluster's template are predictions of their values at the sample site.

Report panel

The *Report panel* provides the most comprehensive means for the user to examine the characteristics of any particular cluster in detail. It gives textual and graphical information on the average characteristics of the cluster, including GQA quality class, distributions of trophic levels and feeding groups, physical characteristics of the site, stress types and water chemistry. These data provide a complete profile of the cluster as defined by the archive samples allocated to it during the MIR-max training process. When a new *Input sample* is presented to the system and allocated to a cluster, the information given on the report panel provides pointers to the conditions existing at the site, including predictions of its water chemistry and the likely causes of stress. Thus, the *Report* provides an initial diagnosis of the state of health of the site, and indicates the most likely types and sources of pollution. The final diagnosis may require further field investigation guided by pointers gained from the *Report* and in-depth analysis of the feature maps and templates.

4.5. The Development of Models based on Plausible Reasoning

Introduction to Plausible Reasoning and Bayesian Belief Networks

Traditional expert systems are based on classical logic and operate by the chaining of "If........Then......" rules. These systems are perfectly adequate for diagnostic or prognostic problems involving exact relationships, but have serious weaknesses with respect to combined diagnostic-prognostic problems or problems involving uncertain relationships (e.g. ecological problems). Under conditions of uncertainty it is necessary to employ one of the methods of 'inexact' or plausible reasoning, such as Dempster-Shafer theory of evidence, fuzzy logic or Bayesian inference. The latter has a long history, but was originally considered to be computationally too demanding for use on complex systems. However, this problem was overcome through the development of updating algorithms based on local computations within graphical representations of dependencies (Lauritzen and Spiegelhalter, 1988). This mathematically sound approach, known as Bayesian Belief Networks, now provides the most powerful and consistent means of reasoning under uncertainty. Its great strengths over other methods are that it replicates three important characteristics of human reasoning, namely: a) the ability to reason bi-directionally (i.e. from cause to effect and from effect to cause as required); b) the ability to modify the dependencies between variables whenever new evidence is introduced; and c) the ability to change one's mind when new evidence 'explains away' earlier evidence. These abilities are essential to the development of any general reasoning system (i.e. a system that can reason diagnostically or prognostically as the need arises).

A Bayesian Belief Network (BBN) is a form of expert system in which the knowledge base consists of two distinct parts, a causal network and a set of conditional probability matrices. The causal network defines the 'cause-effect' links between the variables. The conditional probability matrices define the probabilistic relationship that exists between the states of each 'effect' (or child) variable and the states of its 'cause' (or parent) variables. Figure 4.5. shows the causal network of a simple BBN of river ecology. This is presented merely to illustrate the structure of the network, not as a valid working model, so the relationships may appear rather simplistic to experienced limnologists. Each node in the network represents a variable, and the arrows between variables represent cause-effect links and the direction of causality (i.e. from cause to effect)

Each variable has two or more possible states. The conditional probability matrices define the probability of a variable being in each of its possible states, given the states of its parents (i.e. its causal variables). For example, if *Biotope* has two possible states (riffle and pool), *Substrate* has two states (silt/sand and boulder/pebbles) and *Current Velocity* has three states (fast, medium and slow), then the conditional probability matrix for *Biotope* will define the probability of its two states for each of the six possible combinations of *Substrate* and *Current Velocity*. In the case of variables like

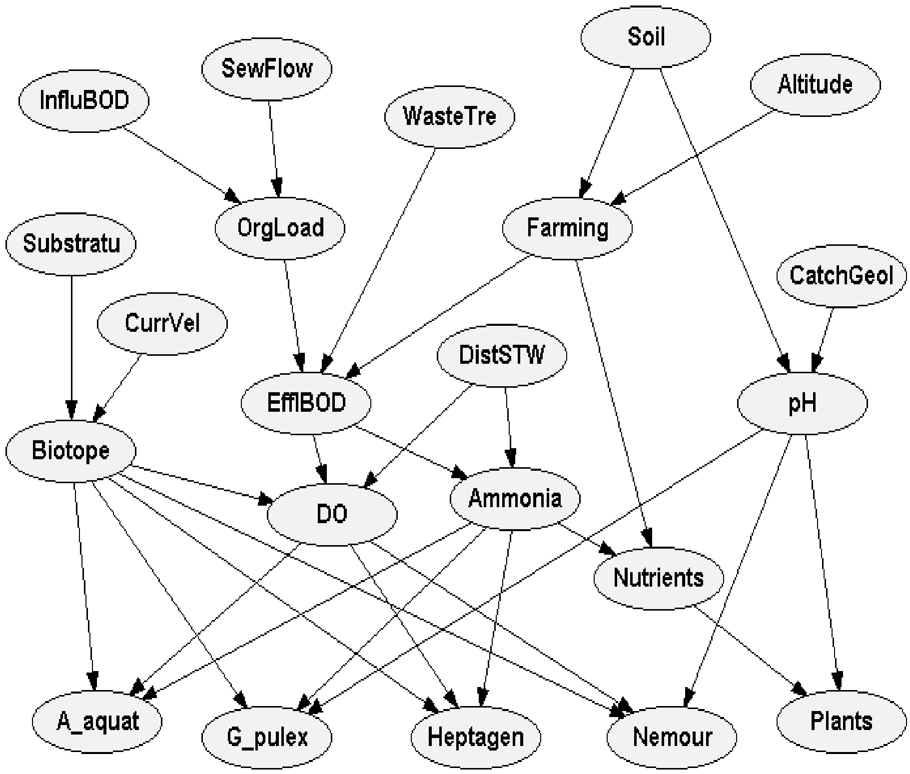

Figure 4.5. The causal network of a simple BBN model of river ecology.

Altitude, that have no parents, their probability matrices reduce to a vector of prior probabilities. The conditional and prior probabilities may be derived subjectively by elicitation from experts or more objectively by data analysis, if a suitable database is available.

In the absence of any evidence about the state of the system, the likely states of the variables are equal to their prior probabilities. When evidence is presented to the network, in terms of the observed state of one or more of its variables, the beliefs in the states of all the other variables are updated using algorithms that are soundly based in probability theory.

Commercial Software for the Development of BBN Models

There are two leading commercial software packages for the development of Bayesian Belief Networks, namely HUGIN and Netica. For many years HUGIN was the clear leader in the field, but recent improvements to Netica have made it a very strong challenger for the top spot, especially if price is taken into account.

Both have user-friendly interfaces for the development and exploration of what might be termed ‘example networks’. However, the construction of a more complex model for use in a real-world setting necessitates the development of a purpose-designed interface. This requires programming skills and various Application Programmer Interfaces (API) are supplied for this purpose with the top-of-the-range HUGIN and Netica packages. Basic details of the main commercial and educational packages available (as of April 2003), together the web addresses of the suppliers are given below in “Summary of Development Systems and Operational Models”.

4.6. RPBBN: An Operational ‘River Pollution Bayesian Belief Network’

RPBBN was developed for the Environment Agency of England and Wales as part of National R&D Research Project E1-056 (Walley *et al*., 2002). The database used for its development was derived from the 1995 survey of rivers in England and Wales, and consisted of spring and autumn samples for 3615 sites having biological, environmental and chemical data. The chemical data listed for each site and season were the average values over the three months prior to the date on which the biological sample was taken.

The Causal Network

The causal network used for RPBBN is shown in Figure 4.6. It has three levels of

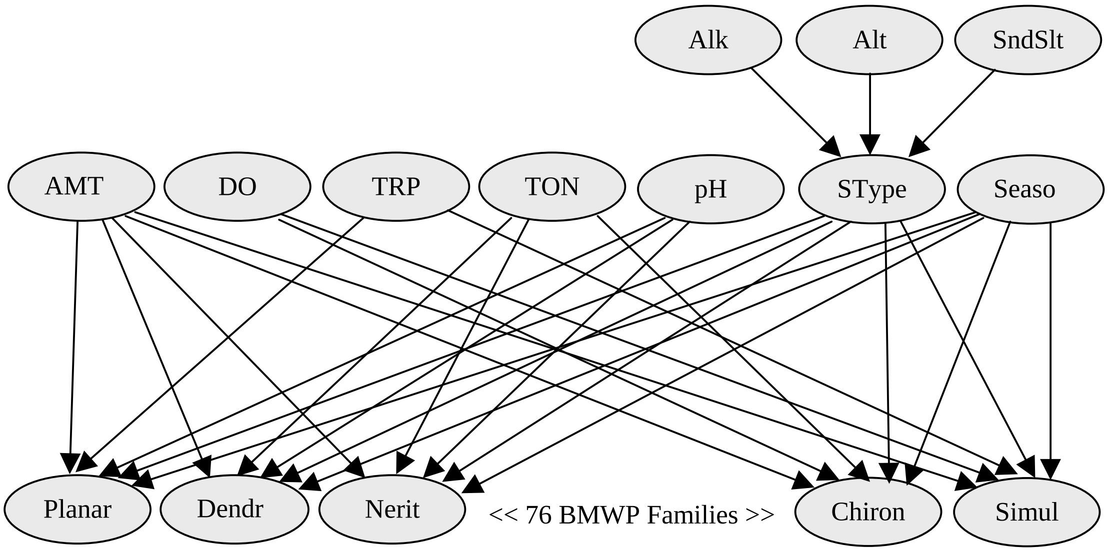

Figure 4.6. The causal belief network of RPBBN

dependency: 76 child nodes (i.e. the BMWP families with 4 possible states – absent and 3 abundance levels), seven parent nodes (i.e. five chemical variables, *Site Type* and *Season*) and three grandparent nodes (i.e. *Alkalinity*, *Altitude* and percentage *Sand+Silt* – all parents of *Site Type*). The five chemical variables were total ammoniacal nitrogen (*AMTN*), dissolved oxygen (*DO* – percentage saturation), total reactive phosphorus (*TRP*), total oxidised nitrogen (*TON*) and *pH*. *Alkalinity*, *Altitude*, *Sand+Silt* and the five chemical variables all had five states each, whereas *Site Type* had three and *Season* had just two (i.e. spring and autumn). The site types were based on work by Walley *et al.* (1998) who classified the 3615 sites in the database into five types, varying from upland fast-flowing riffles (type 1) to lowland slow-flowing 'pools' (types 5). The three states of *Site Type* consisted of types 1-2, types 3-4 and type 5.

Ideally, each of the 76 biological variables should have been linked to each of the seven causal variables above them, but if this had been done their conditional probability matrices would have required the derivation of 75,000 probabilities (i.e. the product of the number of states of the child node and the parent nodes = 4×5×5×5×5×5×3×2) from just 7,230 samples. This was clearly not viable, despite many of these probabilities being equal to zero because they represent 'impossible' combinations of states. So, it was decided to reduce the size of the conditional probability matrix by reducing the number of chemical variables linked to each family from five to three, thereby reducing the size of the conditional probability matrices to 3,000. The links that were retained were determined by using mutual information to identify the chemical variables that had the most influence on the well-being of each family (Walley *et al*., 2002).

The Conditional Probability Matrices

The conditional probability matrices were derived from the data, and then smoothed using purpose designed software (DITHER) developed by CIES. The aim of the smoothing procedure was twofold: a) to smooth out the 'lumpiness' of the raw probability distributions and thereby produce distributions closer to the true underlying distribution; and b) to replace any zero probabilities by small positive values. The latter is equivalent to making the system sceptical about claims that some things either never or always happen. It has the effect of improving the overall performance of the system and making it more robust to extreme cases and marginally erroneous data.

Functionality and User Interface

The graphical user interfaces of BBN development software, like HUGIN and NETICA, are only suitable for demonstrating simple example networks. For a real-world problem, it is necessary to develop a purpose designed user interface. Figure 4.7 shows the main screen of the interface that was designed for RPBBN.

The user enters data from file through a data selection screen (not shown), which is accessed via the *Record Selector* button at the top of the main screen. Once selected, full details of the site and its recorded data are displayed in the *Sample Record Data* panel in the bottom right side of the main screen. The user can then choose to enter all the known biological data and/or the environmental/chemical data using the *Enter Taxa Data* and/or *Enter Environmental Data* buttons at the top of the main screen. These data are then displayed in the *Biological Data* and *Environmental and Chemical Data* panels respectively. In the example shown in Figure 7, the user has entered all of the biological sample data plus *Season*, *Alkalinity*, *Altitude* and

Sand+Silt. In the *Biological Data* panel, the abundance levels of the taxa found in the sample are indicated by black bars on the abundance level bar charts, whereas the absent taxa are indicated by a cross in a small box. If the user clicks on the small box, a bar chart is displayed indicating that the taxon is absent, as illustrated by Elmidae in Figure 7. By double clicking on any one of the black bars, it will be replaced by a probability distribution (i.e. similar to that for 'Oxygen % Saturation' in Figure 4.7.) showing the most likely abundance level of the particular variable, given the current state of evidence on all the other variables. Thus, one can check whether the recorded value of any variable is consistent with the rest of the evidence. This provides a powerful means of identifying potential errors in the data, and thus offers a sound basis for a quality assurance procedure.

Figure 4.7 shows a typical diagnosis, in which the state of health of a river, as defined

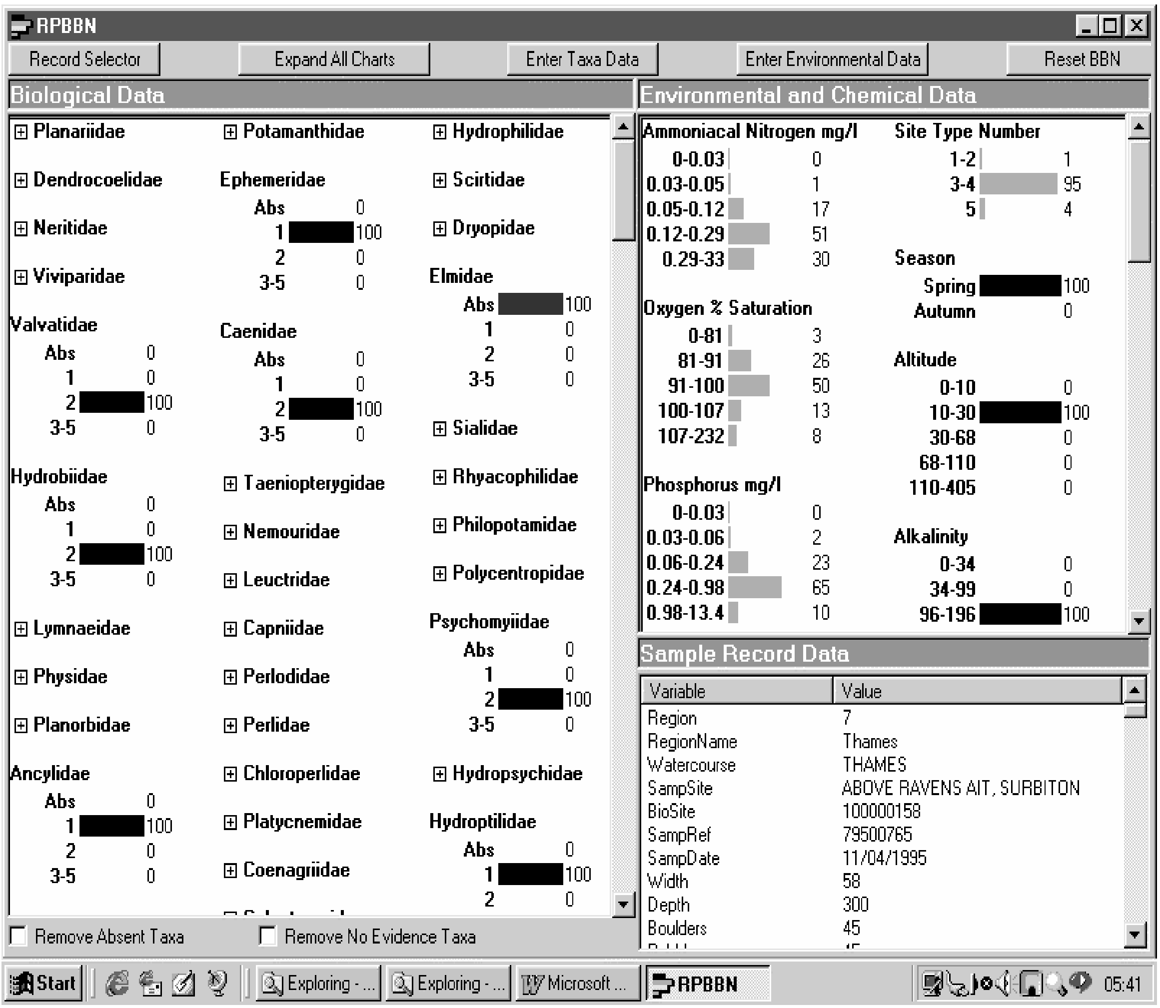

Figure 4.7. The main screen of the RPBBN user interface showing a typical example of the prediction of chemical variables from recorded biological and environmental data.

by a limited set of chemical variables, is being predicted from biological and environmental data. The predictions indicate that *Ammoniacal Nitrogen*, *Oxygen % Saturation* and *Phosphorus* are probably in the ranges 0.12 to 0.29 mg/l, 91% to 100%; and 0.24 to 0.98 mg/l respectively. In fact, the recorded values were 0.28 mg/l, 104% and 0.51 mg/l respectively. To view the predictions for *Total Oxidised Nitrogen* and *pH*, the user has to scroll down the *Environmental and Chemical Data* panel.

Since RPBBN is a diagnostic / prognostic model, it can also be used to predict the change in community composition resulting from changes in water chemistry. In this case, the user would enter all of the known chemical and environmental data. This would produce a prediction of the biological community in probabilistic terms. The user could then modify the values of the chemical variables to reflect those expected after completion of improvement works (i.e. a programme of measures), for example. Double clicking on the appropriate bands in the probability bar charts of the chemical variables can do this. The probabilities of each taxon would then be updated to indicate the predicted new community structure.

Although the user interface of RPBBN provides some very useful functions and clearly demonstrates the potential of BBN models for use in relation to the WFD, it is clearly not as fully developed as that of RPDS. However, it is now being further developed as part of a new Environment Agency contract, aimed at extending the functionality of RPBBN and RPDS in relation to the WFD.

4.7. Tests on AI-based Models

RPDS and RPBBN

During the development of RPDS and RPBBN, several workshops were held with Environment Agency staff to test and review the design of the user interface. Before delivering the models for field-testing, a workshop was held with potential end-users to test the utility and user-friendliness of the models Their responses were very positive and encouraging. The final versions of the models were delivered to the Agency in October 2002, and feedback since has also been very positive.

Although the opinions of experienced river managers and field biologists provide a valuable assessment of the operational worth of the models, their overall performance is best judged by tests on independent field data. National surveys of rivers in England and Wales are carried out every five years. Since RPDS and RPBBN were developed using the 1995 survey data, it was intended to test them on the 2000 survey data. However, these data were still not available to CIES at the time RPDS and RPBBN were delivered to the Agency. Consequently, they were tested on the 1995 data. This was not ideal, but since RPDS was an unsupervised-learning model the tests were not strictly dependent, because the chemical data (the subject of the prediction) did not contribute to its training. In the case of RPBBN, two-way cross-validation was used to perform independent tests. Under a current EA contract RPDS and RPBBN will still be tested on the 2000 Survey data.

Results of Tests on RPDS 2.0

Rank correlation coefficients (r_S) between the predicted and actual values of 34 chemical variables ranged from 0.854 for total calcium (mg/l) to 0.345 for total iron (mg/l), but 11 had r_S values greater than 0.75. Total oxidised nitrogen, non-ionised ammonia, pH and total reactive phosphorus had r_S values of 0.763, 0.700, 0.685 and 0.663, respectively. One of the poorest results was for dissolved oxygen (% sat) which only achieved an r_S values of 0.394. A comparison between river quality classifications based on RIVPACS and equivalent classifications based on RPDS showed that 77 percent agreed exactly and 93.7 percent were within one class interval of each other. Full details of these test results were reported by Walley *et al*. (2002).

Results of Tests on RPBBN 1.2

The rank correlation coefficients achieved in the independent tests were: total ammoniacal nitrogen (0.501); dissolved oxygen % (0.480); total reactive phosphorus (0.663); pH (0.591); and total oxidised nitrogen (0.656). The equivalent results for the dependent tests were: total ammoniacal nitrogen (0.562); dissolved oxygen % (0.679); total reactive phosphorus (0.701); pH (0.689); and total oxidised nitrogen (0.741).

Comments on Test Results

RPDS was trained on 12,076 samples, whereas the cross-validated RPBBN models that were used to produce the independent and 'dependent' test results were based on 3,615 samples. The very poor predictions of dissolved oxygen may be more to do with when it was recorded than to any inadequacy of the models. Daytime recordings of dissolved oxygen are not as relevant to community structure as the much lower (unrecorded) values that occur at night. It might also be worth modifying the RPBBN model by replacing total ammoniacal nitrogen by non-ionised ammoniacal nitrogen. Better results could be expected if the models were based upon species or genera data rather than family data.

RPD and RPBBN in relation to RIVPACS

RPDS and RPBBN were designed to have a much wider scope and functionality than RIVPACS. RIVPACS was designed to predict reference communities and was later extended to provide classification of ecological status. RPDS and RPBBN were designed as general diagnostic / predictive models for operational use. They were 'trained' on data from all quality classes, and therefore model the whole range of 'clean' and 'dirty' water conditions, not just reference state conditions. Thus, they can predict the community corresponding to any quality state lying within the range of the training data. Their diagnoses distinguish between the various types of impact within a given quality class, and so provide a more refined form of classification than the six-band GQA classification. A more detailed review of the advantages of AI-based models is given below.

Other AI-based based Models

Presently, there are no AI-based models in operational use other than RPDS and RPBBN, but prototype models are being developed and tested by CIES as part of a scoping study funded jointly by EHS in Northern Ireland and EPA in the Republic of Ireland. Separate models are being developed for Northern Ireland and the Republic of Ireland, because the protocols used for the collection of the biological and environmental data are markedly different. This project is due to report its findings in June 2003.

The EU funded project PEAQANN (http://aquaeco.ups-tlse.fr/index2.htm) aimed to develop general methodologies, based on advanced modelling techniques, for predicting structure and diversity of key aquatic communities under natural and man-made disturbances. The techniques developed were based on supervised and unsupervised neural networks to perform predictions and classifications respectively. The models incorporate biological data (i.e. fish, macroinvertebrates and diatoms) plus physical and environmental data from Denmark, Netherlands, Belgium, Luxemburg, France, Italy and Austria. However, it appears that few, if any, of the models were based upon a pooled dataset covering all the countries involved. In view of this and the fact that the datasets from each country were relatively small for neural network modelling purposes, it is clear that the models require further development before they could be of operational value. Since the long-term aim of the investigation is to help define strategies for conservation and restoration, its total dependence on neural network techniques appears unduly restrictive.

4.8. Advantages and Uses of AI-based Models

MIR-max Models

MIR-max is a holistic pattern classifier with powerful data visualisation functions. It was originally designed for use with ecological data, but is suitable for use on pattern recognition problems in any field. Its holistic nature means that classification and data interpretation are based on the community composition as a whole, not on a hierarchical process based on the presence or absence of key indicators. Thus, it is less prone to error when used under conditions of uncertainty. In addition, it means that the model is based upon data from all river types and quality classes, thus when it diagnoses the state of health of a site (i.e. predicts chemical variables, likely stresses and quality class) it does not have to extrapolate outside its training data, unlike quality classifications based upon reference state models (e.g. RIVPACS).

Data Requirements

At present, MIR-max requires that the input data for training and classification purposes are complete (i.e. no missing values). However, a new version has been developed, but not yet fully tested, which allows the classification of samples having some missing data. There is no requirement concerning the amount of data necessary to train a MIR-max model, but the number of output classes used is limited by the number of examples (samples) in the training data set. A general rule-of-thumb is that the number of classes used should not exceed one tenth of the number of example.

MIR-max accepts a variety of data input formats, including comma, space and semicolon separated text files, all of which can be generated from standard spreadsheets and/or databases. The default format is comma separated (.csv).

Each input variable must be either binary (0, 1), discrete ordinal (e.g. abundance categories 0, 1, 2, 3, 4) or continuous values (e.g. pH). There is no requirement for the ordinal or continuous data to be interval-valued (as is the case with classifiers based on a Euclidean similarity metric). Since MIR-max is a discrete model, the continuous valued data have to be transformed to a set of discrete ordinal bands. This is done during the construction of the indicators file. Nominal data (e.g. Colours: Red, Green, Blue) can be included in the input as separate binary variables (i.e. 0 for absent or false and 1 for present or true).

User Friendliness

MIR-max has a user-friendly interface and a comprehensive user manual. New users with moderate computer literacy can learn to develop models from their own data with little difficulty.

Potential Uses

MIR-max has many potential uses that are directly relevant to the WFD.

- Diagnosis of the ecological status of waterbodies from biological and environmental data. This was the use for which it was originally designed. When used in this way, new samples are classified to a particular cluster and the reporting function provides a set of predictions of the river's chemistry and its likely stresses. When used by experienced limnologists, the data visualisation aids (i.e. the feature maps and templates) often help to refine the diagnosis. The RPDS model is a good example of this type of use.

- Biological classification of river or lake quality. Once a diagnostic model has been developed, it is a small step to classify an individual diagnosis into a five-band classification system. This is clearly possible because a diagnosis (e.g. into one of 100 or more classes) is simply a more refined form of classification (e.g. into one of five bands). The advantage of this approach to classification is that it is not dependent upon a pre-defined set of reference sites, since the MIR-max diagnostic model uses data from all sites, irrespective of their quality. Such classifications can, however, be made to relate to reference states.
- Prediction of the ecological impact resulting from changes in the chemistry and/or physical characteristics of waterbodies. In this case the MIR-max model is trained using the chemical and environmental data, and a new input case (i.e. a chemical/environmental scenario) is classified to a specific cluster. The reporting function then provides a prediction of the ecological state corresponding to the particular input case. Thus various scenarios can be tested to determine their impact, for better or worse, on the ecology of the river (or lake).
- Definition of physical or biological typologies. If MIR-max is presented with input data consisting only of the physical (or environmental) characteristics of river or lake sites, the resulting clusters will be a set of *site types*. If biological data from reference or 'clean' sites are used as input, then the resulting classes will be a set of reference communities (i.e. a biological typology).
- Identification of potential reference sites. MIR-max diagnostic models cluster sites together based upon their biological and environmental characteristics. Thus those sites that are allocated to the top quality clusters are potential reference sites. All previously defined reference sites should therefore be allocated to one of these clusters. If they are not, their validity as reference sites will be in question. Hence the model provides a means of checking the validity of existing reference sites and of identifying new reference sites.

BBN Models

BBNs are cause-effect models of a system, and in this respect they are similar to process models. However, process models only operate predictively (i.e. from cause to effect) whereas BBNs operate predictively or diagnostically (i.e. effect to cause) as and when required. In addition, they are probability models, so handle uncertainty in a mathematically sound and consistent way. Thus they are ideal for modelling the knowledge-based reasoning processes that experts use to solve complex problems of diagnosis or prediction (or prognosis). However, BBNs cannot model continuous time-varying processes, especially cyclic processes, as readily as process models. Although most BBNs are discrete models, it is possible to construct continuous models, but this involves representing the multi-dimensional conditional probability matrices by multi-dimensional continuous probability functions, which is generally not practical. The main problem that can arise with BBNs is that conditional probability matrices can become excessively large if a node has many parent (i.e. causal factors). This is not a problem for the software, but for the reliable estimation of the probabilities, unless the database is very large. However, one should be careful before concluding that this is a weakness of the BBN modelling technique. In fact, it brings modellers face-to-face with the important reality that they may have insufficient information (knowledge or data) to adequately represent the complex behaviour of the systems they are attempting to model. This is often not realised when using statistical or black-box techniques, like neural networks, which simply fit a model to the data. In reality, if there are insufficient data to build a BBN model, then it is likely that there are insufficient data to build a truly representative model of the system using other modelling techniques. One of the great strengths of the BBN approach is that it allows the imposition of a structure on the model that conforms with current scientific knowledge of the structure and behaviour of the system. This makes the model far more robust and less likely to produce erroneous conclusions. It also enables developers to incorporate both scientific knowledge and information from data into their models, thus making maximum use of available information resources.

Once created, a BBN provides a single all-purpose model of the system, similar to, but no doubt simpler than, that held in the minds of experts. Thus, the user can present any snippet of evidence to the model, anywhere in its structure, and the model will update its predictions of the states of the other variables in the network, but in doing so it will only modify those variables to which the evidence is relevant (i.e. the dependent variables). In reality, the dependencies between variables change whenever new evidence is introduced. One of the great strengths of the BBN method over other methods of reasoning is that it automatically modifies the dependencies every time new evidence is added. This, together with its ability to reason bi-directionally on every cause-effect link, results in reasoning that is mathematically sound and consistent.

It is worth noting that commercial BBN development packages, like HUGIN and Netica, offer developers the ability to create BBNs entirely from data. That is, the system generates both the causal structure of the model and its conditional probability matrices through analyses of the database. This sounds very attractive, but in fact it often leads to causal structures that do not conform with expert opinion. The most likely reason for this is that databases do not, in general, contain all of the variables that are relevant to the model. If some are missing, then the causal structure created by the software will be distorted in some way, and hence erroneous. This approach also fails to utilise the most valuable information sources with respect to the causal structure, namely scientific knowledge. It also requires the use of a single database, thus undermining the benefits to be gained from the use of multiple databases, as explained below.

Another important advantage of BBNs is that they are very easily modified. If one wishes to add an extra node (variable) anywhere in the network, it only involves the derivation of its conditional probability matrix, and the revision of the matrices of any existing variables to which the new node has become a parent (or causal variable).

Data Requirements

The format of the data required for the development and use of a BBN model will depend upon the user-designed interface. The source and amount of data required for development is not limited to one single database, because the conditional probability matrices can be derived from several different databases. This is because the matrix for each variable only involves probabilities relating to the variable itself and its parents (i.e. its immediate causal variable). Thus, different databases (perhaps even from different counties) can be used for each variable, provided they include data on the variable and each of its parents. If it is intended to use software to derive the entire causal structure of the network from data, then data on all of the variables will have to appear in a single database.

User Friendliness

The development of a simple BBN is very easy using the graphical interface of a commercial software package, like HUGIN and Netica. However, the development of a BBN for a complex real-world problem requires the necessary programming skills to use an API to build a bespoke user-interface.

Potential Uses

BBNs have considerable potential for use in relation to the operational tasks associated with the WFD. A fully comprehensive BBN covering the range of factors indicated in Figure 4.5, would open up the possibility of having an outstandingly knowledgeable and highly consistent expert limnologist in every office. This expert would be able to predict the state of every variable in the system, given the states of any subset of those variables. Thus users would be able predict, for example, the effects on the biological community of any changes in water chemistry, provided the chemical variables in question formed part of the model. Alternatively, users could predict the water chemistry from the biological community, or the impact of a change of land use on say pH or eutrophication. However, the construction of such a comprehensive BBN might take years to develop, because of the need to acquire suitable databases for different parts of the model. However, the ease with which BBNs are modified makes incremental development of such as system not only viable but, indeed, a particularly attractive proposition.

4.9. Summary of Development Systems and Operational Models

MIR-max

Type: Software for the development of MIR-max models (e.g. RPDS).

Applications: Diagnostic / prognostic models for rivers and lakes.
Development of typology classifications.

	Identification and validation of potential reference sites.
Data requirements:	No minimum size requirement.
	Delimiter – comma, semi-colon, space or user defined.
	File extension – .txt, .csv, .skv or user defined.
	Decimal point format – US/UK (e.g. 45.2) or European (45,2).
Available system:	MIR-max 0.2 Price: Free (plus £10 handling charge).
Platforms:	Windows 98/NT/2000/XP.
Supplier:	Centre for Intelligent Environmental Systems.
Suppliers web page:	http://www.cies.staffs.ac.uk
E-mail contact:	m.a.oconnor@staffs.ac.uk or w.j.walley@staffs.ac.uk

HUGIN

Type:	Commercial software for the development of BBN.	
Applications:	Plausible reasoning models of any type of system, including any type of ecological system or water resources system.	
Data requirements:	No minimum size requirement.	
	File formats depend on the user's design of the interface.	
Available systems:		
Commercial	HUGIN Developer (includes APIs).	Price: €6310
	HUGIN Explorer	Price: €3150
Educational	HUGIN Researcher (includes APIs)	Price: €1720
	HUGIN Educational	Price: €850
Demonstration	Free via web page (system has limited capabilities).	
APIs	C, C++, Java and an ActiveX-server for e.g. Visual Basic.	
Platforms:	Windows 98/NT/2000/XP, Solaris 7 or 8, Linux Redhat 7.0.	
Supplier:	HUGIN Expert.	
Suppliers web page:	http://www.hugin.com	

Netica

Type:	Commercial software for the development of BBN.
Applications:	Plausible reasoning models of any type of system, including any type of ecological system or water resources system.
Data requirements:	No minimum size requirement.

	File formats depend on the user's design of the interface.
Available systems:	
Commercial:	Price: €550
Educational/Personal:	Price: €268
Demonstration	Free via web page (full-featured but limited in model size)
APIs:	C, C++, Java, Visual Basic (Microsoft platforms only)
Suitable platforms:	MS Windows or Macintosh
Supplier:	Norsys
Suppliers web page:	http://www.norsys.com

RPDS 2.0

Type:	Model for the diagnosis of river health in England & Wales.
Current user:	Environment Agency, United Kingdom.
Applications:	Prediction of pollutants and likely sources from biological and environmental data. Water quality information system.
Data requirements:	Data input may be from Excel (.csv file) or manual input.
Available system:	RPDS 2.0 Price: Free (plus £10 handling charge)
Platforms:	Windows 98/NT/2000/XP
Supplier:	Centre for Intelligent Environmental Systems
Suppliers web page:	http://www.cies.staffs.ac.uk
E-mail contact:	m.a.oconnor@staffs.ac.uk or w.j.walley@staffs.ac.uk

RPBBN 1.2

Type:	Model for the diagnosis / prognosis of river health in England & Wales.
Current user:	Environment Agency, United Kingdom.
Applications:	Prediction of Ammonia, DO, TRP, TON & pH and from biological and environmental data. Prediction of the effect of remedial works or increased pollution on the composition of the macroinvertebrate community.

	Quality assurance of biological samples.
Data requirements:	Data input may be from Excel (.csv file) or manual input.
Available system:	RPBBN 1.2 Price: Free (plus £10 handling charge)
Platforms:	Windows 98/NT/2000/XP
Supplier:	Centre for Intelligent Environmental Systems
Suppliers web page:	http://www.cies.staffs.ac.uk
E-mail contact:	d.j.trigg@staffs.ac.uk

CHAPTER 5 GROUNDWATERS

5.1. Requirements of the WFD with respect to groundwater modelling

The integrated catchment approach of the implementation of the WFD requires viewing groundwater as an element of a continuous system, with inputs from precipitation and surface waters, with linkages to surface waters and to ecological systems supported by these surface waters, and to terrestrial ecological systems dependant on groundwater. Identification and assessment of the impact of anthropogenic and natural pressures which act upon and change this system is central to the WFD. This presents challenges in terms of traditional modelling approaches, which have treated ground and surface waters separately and made little or no reference to associated ecosystems. At least in the short term this practice is likely to continue with respect to the implementation of the WFD.

Modelling can be employed to help with many aspects of the requirements of the directive as it relates to groundwater. It can assist with *Initial Characterisation* of groundwater bodies in each River Basin District (Article 5 and Annex II 2.1, Groundwaters). This includes:

- Delineation of groundwater bodies, and identifying linkages to directly dependant surface water bodies, associated surface water ecosystems and associated terrestrial ecosystems;
- Identification of pressures to which the groundwater bodies are liable to be subject and an assessment of the degree to which they are at risk of failing to meet environmental objectives for ground and associated surface waters and ecosystems as defined in Article 4 and Annex II; and
- Assessment of the uses of the water bodies

Further Characterisation is required for phase groundwater bodies identified as being at risk is required, in order to establish a more precise assessment of risk and identify Programmes of Measures (Article 11 of the WFD).

5.2. Characterisation of Groundwater bodies

5.2.1. Delineation of groundwater bodies in Ireland

Delineation of groundwater is specific to Irish hydrogeological conditions and although modelling will only play a small role in delineation, the interpretation of the WFD is key in the uses of modelling at other stages of implementation.

The WFD defines:

- Groundwater as *"all water which is below the surface of the ground in the saturation zone and in direct contact with the ground or subsoil"*;
- Aquifer as *" a subsurface layer or layers of rock or other geological strata of sufficient porosity and permeability to allow either a significant flow of groundwater or the abstraction of significant quantities of water";* and
- body of groundwater as *" a distinct volume of groundwater within an aquifer or aquifers"*

The Irish Groundwater Working Group (2001) considered that a "Groundwater Body" should be of sufficient size to provide for the substantial abstraction of significant quantities of water; and connection of groundwater with ecosystems can put them at risk, either through the transmission of pollution or by unsustainable abstraction that reduces baseflows. Groundwaters should be managed to prevent environmental impacts on surface ecosystems.

The Groundwater Body is, therefore, the management unit into which large geographical areas of aquifer can be subdivided. Equally, aquifers may be grouped to form groundwater bodies. All groundwater bodies will, therefore, constitute part of an aquifer or aquifers.

Under the aquifer categories defined in *Groundwater Protection Schemes* (DELG/EPA/GSI, 1999), which will be used initially to delineate of groundwater bodies, all Irish bedrock units are defined as aquifers, along with subsoil classified as sand/gravel. Aquifer are based on productivity, lithology, hydrogeology and structure.

However, groundwater bodies to be delineated under the WFD are restricted to regionally important aquifers (karst Rk, fissured bedrock Rf and extensive sand/gravel Rg), and locally important sand/gravel (Lg) and bedrock which is generally moderately productive (Lm). The main aquifers in Ireland are Carboniferous and older bedrock ones characterised by fissuring, some limestone formations with well developed karst, and Quaternary sand and gravel deposits (Misstear, B. *et al*, 1999).

The delineation of groundwater bodies will largely coincide with surface water catchment boundaries, which generally appear to match sub-surface boundaries and link with surface ecological systems.

In the context of the WFD, "overlying strata" are the geological materials overlying the water table in unconfined groundwater bodies and overlying the top of the geological unit forming confined groundwater bodies. Both these strata and the aquifer type may need to be taken into account in the construction of a conceptual model of groundwater body or bodies.

Apart from sand and gravel, aquifers categorised in *Groundwater Protection Schemes* (DELG/EPA/GSI, 1999) refer only to water within bedrock aquifers moving by saturated flow. Unconfined flow in subsoils above the bedrock surface is not included. The water bodies defined on the basis of these aquifers do not, therefore, with the exception of sand and gravel aquifers, include saturated flow in the subsoil. This is an interpretation, in light of Irish hydrogeological conditions, of the definition in Article 3 of the WFD of *"Groundwater" as all water which is below the surface of the ground in the saturation zone and in direct contact with the ground or subsoil*.

Groundwater bodies are the basic unit to which groundwater modelling is applied. They will always be regarded as one element of the hydrogeological system of which they are part.

5.2.2. Modelling in the Characterisation process

During the Initial Characterisation phase, only existing hydrogeological and geological data will be available. The roles for modelling will therefore be restricted. It is also assumed that professional geological and hydrogeological judgement will be used to carry out much of this initial characterisation.

Further characterisation is to be carried out on groundwater bodies identified as being at risk of failing to meet environmental objectives during the initial characterisation process. This is carried out in order to establish a more precise significance of such risk, so as to identify what measures need to be taken. The level of characterisation specified in the WFD is detailed and there is a clear role for modelling. The type of characterisation required is, however, inextricably linked with the evaluation of the pressure upon the waterbody, the resulting state of the waterbody and impacts upon it or linked ecosystems. The integration of characterisation and pressure-state, state-impact evaluation occurs at a number of levels. It occurs at a hydrogeological process level and at a technical modelling level, where flow system characteristics are required *a priori* information for modelling of pollutant transport. In addition, a characteristic of the groundwater body such as water level, can also represent a pressure upon a dependant ecosystem such as a fen.

5.3. Identification and estimation of Pressure- State relationships

The identification of anthropogenic pressures on waterbodies forms part of the initial characterisation process, with more precise estimate of any risk identified during further characterisation.

For both surface and groundwaters risk assessment plays a key role in the implementation of the WFD. Risk incorporates both the probability of occurrence of an event and the magnitude of the harm caused. Two frequently used methodologies, often in some combination, are the traditional toxicological source-pathway-receptor approach (U.S. E.P.A, 1989), and that adopted by the U.K. Department of the Environment (Department of the Environment, 1995). Risk methodology describes the same sequence of events as that described by the Drivers, Pressures, State, Impact, Response model (DPSIR), but with an emphasis quantitative measure of probability of occurrence.

A risk analysis methodology describes a *Driver* which produces a Hazard or *Pressure*, a pathway, and a receptor, upon which *Impact* or harm occurs. The impact on the receptor is a combination of the *State* (or probability of the state) of the waterbody, the nature of the receptor and what constitutes harm to that receptor. Harm is, broadly, a failure to achieve the environmental objectives.

Pressures on groundwater bodies and their associated systems, for which the relationship between pressure, and state (or probability of state) at a specified receptor, can be estimated using modelling techniques that address:

- Changes in water levels (groundwater hydraulic head) owing to abstraction for industry, public or private supply;
- Point source contamination including from historical contaminated land, mining or waste disposal; and
- Diffuse sources of pollution, predominantly nutrients from land-use activities.

Pathways linking pressure-state-impact relevant to groundwater can be wholly internal, or through a link with surface waters, and associated ecosystems. As with surface waters, the use of a reference condition defines acceptable groundwater quantitative or chemical status. Consequence of this in surface water ecology or, perhaps directly, on drinking water standards defines the impact. Table 5.1. lists receptors for which consequences can potentially be estimated using modelling.

Table 5.1. Receptors for which state/probable state can be estimated by modelling with groundwater threshold or values.

Receptor	Impact constitutes a negative change relative to defined thresholds as defined below
Groundwater body	Quality standards to be defined by EU under Article 17 currently the Draft Directive Com(2003) on the protection of groundwater against pollution Quality standards under other EU legislation No evidence of saline intrusion Quantitative standard of level such that available groundwater resource is not exceeded by long term average abstraction. No alterations in flow associated with saline intrusion Upward trend in pollutants, baselines to be defined under Article 17 currently the Draft Directive Com(2003) on the protection of groundwater against pollution
Water bodies used for or likely to be used for Drinking Water Abstraction As defined in Article 7	Drinking Water Directive quality standards
Linked Surface Water Bodywith associated ecological system. In the Irish implementation of the directive only proposed or designated SACs, SPAs and NHAs are to be considered.	Surface water quality standards Quality standards supporting current/good ecological status Quantitative standard supporting current/good ecological status
Terrestrial ecological system directly dependant on ground water. In Ireland these comprise wetland ecosystems and only SACs, SPAs and NHAs are to be considered	Quality standards representing current/good ecological status Quantitative standards representing current/good ecological status
Nitrate Vulnerable zones	Quality standards as in Art.4(1)c
Urban Waste Water Directive sensitive zones	As defined in the Urban Waste Water Directive

The most recent draft document produced by the Irish WFD Groundwater Working Group confirms this risk based approach to pressure-state-modelling (Figure 5.1).

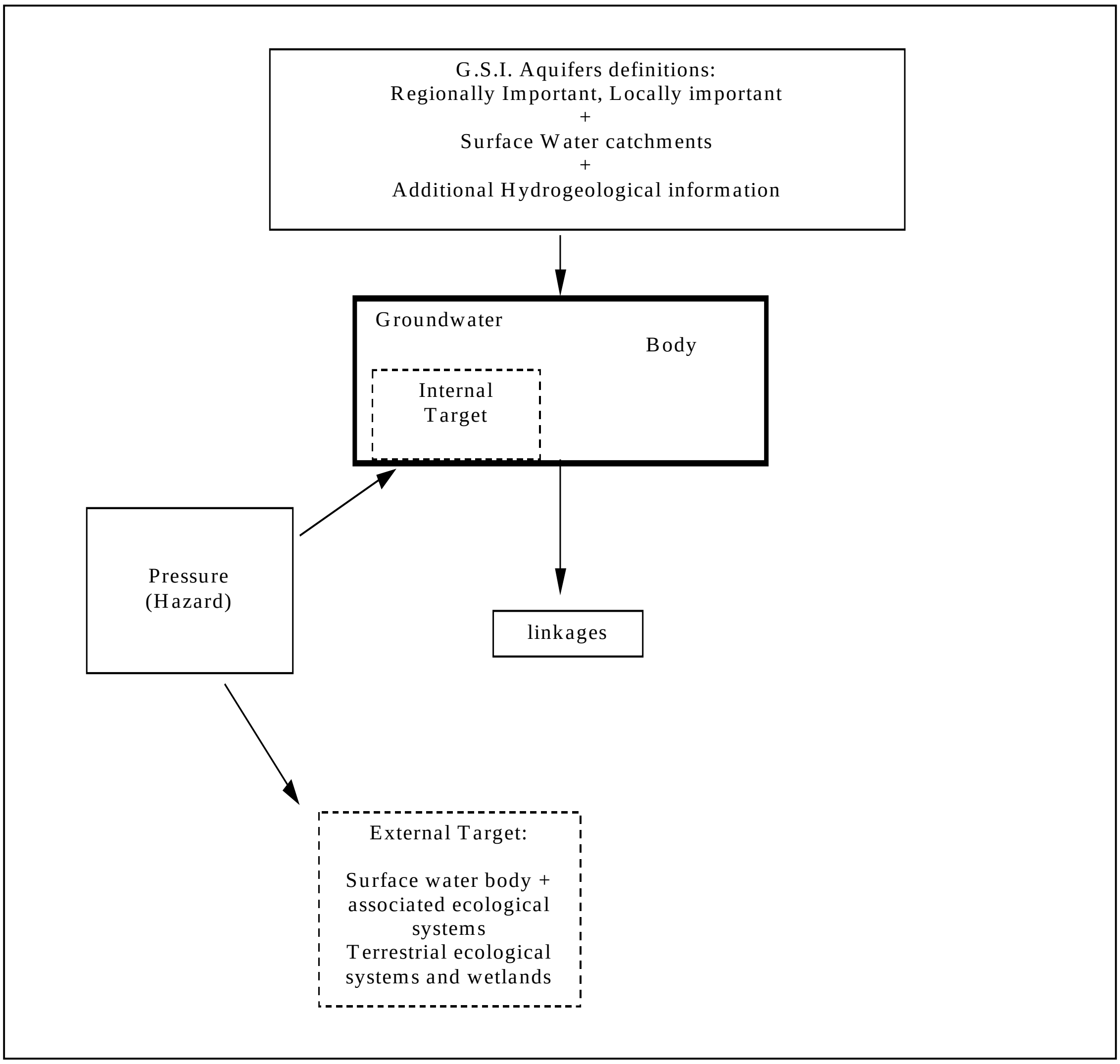

Figure 5.1. Outline Risk Approach to Groundwaters

5.4. Initial assessment of pressures and their risk to groundwater bodies

In terms of the initial assessment of risk to groundwater bodies, the existing Geological Survey of Ireland (GSI) assessment of groundwater vulnerability provides a qualitative methodology. Approximately half of the country has been assessed for vulnerability under this scheme. This system is risk-based within a hazard-pathway-receptor framework. The hazard is provided by the pollutant activity and depends on the contaminant loading. The pathway, and a qualitative probability are combined in the groundwater vulnerability measure. Vulnerability is based mainly on the thickness and permeability of the subsoil, though the type of recharge (diffuse or point, the latter occurring via karst features) and, for sand and gravel aquifer, presence of an unsaturated zone. The receptor is provided by the aquifer (the groundwater resource) and by the presence of a major water supply well or spring (the source). The consequences of the contamination hazard depend on the value of these receptors (Misstear *et.al*., 1999). It is not envisaged that any specific pressure-state models would be developed for this process.

5.5. Modelling for Initial and Further Characterisation and Pressure-State Estimation

Modelling pressure-impact will have a limited role in initial characterisation but an extensive role in further characterisation and in the more precise estimation of risk to waterbodies. The traditional focus of groundwater modelling has been the simulation of the response of groundwater hydraulic heads to changes in abstraction or recharge and contaminant transport based on flow models. In implementing the WFD, this focus will have to expand to include consideration of pressures on linked surface waters and surface water and terrestrial ecosystems, and integration of risk estimation within the modelling framework.

Groundwater models which apply to characterising groundwater systems (consisting of groundwater body(ies) and linkages) and to estimating pressure-state relationships fall into two categories (Peck *et. al*., 1998):

- *Identification or Evaluation Models,* which may be used to identify the parameters and boundaries of a poorly understood aquifer or hydrogeological system. Calibration is used to define model parameters and boundaries including pollutant distributions. This type of modelling is applicable for characterisation of water bodies, identification of linkages, and estimates of pressure caused by groundwater head and flux and pollutant load.

- *Prediction Models,* which predict the response of a groundwater system to variation in hydraulic heads, and natural and/or artificial hydraulic stresses. distribution of a contaminant can be predicted. This type of modelling is applicable to the estimation of risk to ground and surface waters quality from potential pollutant or abstraction pressures. Predictive modelling is also valuable in the identification of remedial response and success of a Programme of Measures.

See further discussion on initial characterisation in section 5.15 and further characterisation in section 5.16.

5.6. Choice of Model

The uses of modelling to assist with implementation of the WFD are varied, depending on specific objectives. As outlined in Chapter 1, modelling for clearly defined groundwaters, as for surface water bodies, require a good conceptual model of the flow system and processes involved. The purpose(s) of the model and the conceptual model will determine what type of governing equations are used in a mathematical model and what computer code will represent them. Availability of appropriate data dictates the modelling approach. Variables of interest include hydraulic head, flux and contaminant concentration. Choices are also made depending on whether a single value of a variable, or a distribution of results across a problem domain are required. The remainder of this section discusses issues relevant to the choice of groundwater model. Similar issues apply to many other domains. See also Riza/Stowa (1999) and discussion of good modelling practice outlined in Section 1.5.

5.7. Purpose and Scale

The purpose and scale of groundwater models are strongly interrelated. Processes may vary from simple one or two-dimensional flow in a waterbody to three dimensional transport of pollutants. Groundwater models may be developed to solve problems at widely different spatial scales, from local scale (e.g. one or two dimensional simulation of flows within a 10 m radius of a well) up to regional or catchment scale three-dimensional simulations of flows. Modelling at a variety of different scales will be required to achieve the requirements of the WFD. Good definition of the scale requirements and implications of each model is extremely important.

5.8. Representation of the Flow System

Representation of the flow system has two main aspects, a) the level of representation of the model and b) the conceptualisation of the groundwater system.

Level of Abstraction of the representation

Level of abstraction refers to the degree to which the processes occurring in the system are explicitly represented in the model.

- *Conceptual models* represent the largest degree of abstraction.
- *Stochastic models*, relate hydrogeological variables to one another by statistical methods, but with no representation of the process involved in the relationships.
- *Black-box models*, relate generally to the relationship between an input parameter to the system and an output parameter, e.g. a linear systems approach deriving a function to relate rainfall input to a point output (discharge) such as a karstic spring.
- *Analytical models*, involves analytical equation or equations that describe some of the processes occurring across a given one to three dimensional distance within the hydrogeological system, and solution requiring information about the system

parameter values. For example, analytical solution of the Darcy equation for flow to calculate discharge from a porous medium at a given location. Analytical models are generally only applied to systems appropriate for modelling in two dimensions since analytical solution of 3-D equations is very difficult.

– *Network Models*, represent the hydrogeological system by a series of links and nodes, which may or may not be referenced to specific locations. The links and nodes refer to given sections of the system with similar properties and/or processes occurring and for which analytical equations, based on the system parameter values assigned to the links and nodes, are solved
– *Distributed models*, require analytical equations that represent processes, solved across a discretised grid by numerical approximation. Numerical approximation allows the solution of more complex equations in three dimensions. The elements of the grid are referenced to specific locations. The process equations are solved for as many locations on the discretised problem domain as there are grid units. System parameter information is required for each unit. Distributed models include finite difference and finite element flow models.
– *Physics based process models* where a number of linked equations for complex processes are solved over a small area. These usually require a large input of system parameter information. These include some large scale nutrient models.

Conceptual method of representing the flow system

The conceptualisation of the groundwater system refers to an understanding of how flow and transport processes in the hydrogeological system occur, and, therefore, the use of the appropriate representation of flow and contaminant transport processes in modelling. There are two main conceptualisations of flow; that described by Darcy's law (Annex 1) and that described by conduit flow (Annex 1). Contaminant transport processes in groundwater include advection, dispersion and chemical reactions.

An important extension of the conceptualisation of flow in porous media by governing equations derived from Darcy's law is that to non-idealised porous media, including fractured media. This is termed the equivalent porous medium (EPM) approach.

Many media have both primary and secondary porosity, in the form of cracks, microcracks, fracture zones, shear zones and weathering fissures. Secondary porosity can exist, from micro- to macro-scales. The EPM approach assumes that fracture apertures and flow velocities are small enough that Darcy's law applies. The primary and secondary porosities are represented by a continuous porous medium having equivalent or effective hydraulic properties. These properties are represented by parameters such that the flow pattern in the EPM is similar to that in the fractured rock. This idea is scale dependant and assumes that for the fractured system there is a representative elemental volume (REV) which is sufficiently large (or small) such that it can be characterised by these effective hydraulic parameter values. Simulation of flow in fractured systems using this method requires definition of effective values for hydraulic conductivity, specific storage and porosity. Working out the scale of area required for the REV is difficult but very important. For example, this approach might be appropriate at regional aquifer scale in a waterbody with secondary porosity at either low or high density, since in both cases an appropriate size REV is available. However, while the high fracture density waterbody may also be modelled at local scale, (since a relatively small REV is required to define effective parameters), the low density waterbody may not suitably modelled at a local scale, since the area to be modelled does not include a sufficiently large REV. The EPM approach is frequently used to represent Irish aquifers which, apart from sand and gravel aquifers, are predominantly bedrock media fractured to some degree. In certain karst areas extreme weathering has resulted in the formation of very large fissures and conduit flow may occur. A system with large fractures can be modelled using the EPM approach where the model domain is sufficiently large to be a REV, and where an estimation of flow at specific points in the fracture system is not required.

5.9. Model characteristics

Number of dimensions to be modelled.

In reality, all groundwater problems are three-dimensional, but three-dimensional modelling has large data and processing time requirements. The practical solution is to reduce the number of modelled dimensions from three to two, but this is only possible where the dominant characteristics of the hydrogeological system can be adequately represented and where the required result can be achieved by this approach.

Probabilistic or Deterministic

The ability to achieve a probabilistic result from a modelling exercise is important for risk estimation and as a way of assessing sensitivity to uncertainty in model parameters. Increasingly, the capacity to achieve probabilistic results from groundwater flow and pollution transport models is being built into commercial software packages. In environment risk estimation, probability has often not been measured, or some qualitative or semi-quantitative measure of probability has been used. Increasingly modelling output provides a probability occurrence (e.g. of a given water level).

The most usual way of producing a probabilistic result in groundwater modelling is by running a Monte Carlo (MC) simulation. Some model parameter is chosen as the random variable upon which the MC simulation is based. The parameter is chosen because it is inherently variable e.g. rainfall (over time) or because there is uncertainty associated with the value e.g. hydraulic conductivity (which is difficult to measure). A distribution for the variable is prepared, either theoretically or derived from statistical analysis of data. The model is then run, with a value from the distribution picked randomly each time a value is required by the model calculations. This process is then iterated, each model run termed a realisation, as many times as is required, usually more that 100 times. Some moment of the result for all of the realisations is then calculated to give the final result. Typically this is expressed as a percentile or confidence value, for example the 95% confidence value. In the case of a distributed model such as a finite difference model, for example, a 95% confidence value of hydraulic head would will be given as a result for each grid square, instead of a single deterministic value for each grid square in the single run non-probabilistic model run. MC simulations have implications for model run time, and for data requirements, where additional data may be required to produce a distribution for the random variable(s) on which the simulation(s) will be based. Monte Carlo simulations are increasingly applied to other domains and are often used to estimate probabilities of exceedance of quality limits, and to guide regulation of pollutant emission loads (See section 3.4.5 [TMDLs] and USEPA, 1999, 2001).

Steady-State and Transient Modelling

Steady-state or dynamic equilibrium conditions occur where the amount of water recharging an aquifer is balanced by an equal amount of discharge and the potential or hydraulic head field is more or less constant over time. When some stress is introduced into a steady-state system, by withdrawal or addition of water, this equilibrium is disrupted and the system will take time to reach a new equilibrium or steady state condition, during which time it is in a non-equilibrium or transient condition. The potential or hydraulic head field is, therefore, time dependant. Under transient conditions, water is released from or taken into storage within the porous material of the aquifer. Heads change with time as a result of this transfer of water. When the transfer to and from storage stops, the system reaches steady state and the heads stabilise. A storage parameter (storativity) must be specified for the simulation. Specific storage (S_s) is used in the three dimensional governing equation (see Representation of the flow system, above), The storage co-efficient (S) is used in two-dimensional areal simulations and specific yield (S_y) is used for unconfined aquifers. Models will require an array of this parameter, one for each node of the grid. Measurement of storativity like many parameters or variables, is subject to error.

When modelling a transient system, the simulation typically begins with steady–state initial conditions and ends before or when a new steady state is reached. Initial conditions refer to the head distribution throughout in the system at the beginning of the simulation. It is standard practise (Anderson and Woessner, 1992) to select as the initial condition a steady state head solution generated by a calibrated model. It is, therefore, necessary to calibrate a steady state version of any model, before moving on to a transient simulation.

A set of time steps is defined for the simulation and the result is a set of heads for each time step. In comparison, steady-state simulations generate only one set of heads. Choosing the appropriate time steps for the model is critical since the values strongly influence the numerical results. The steps may be constrained by the equations solved by the chosen modelling software. The solutions of some equations are prone to numerical instabilities causing unrealistic results, In general flow codes are less prone to this than solutions of the solute transport equation.

Steady state conditions are easier to model than transient ones, since storage parameters are not required and numerical modelling can be more stable. Steady-state is, therefore, often assumed for modelling. Generating a time dependent result, for the purposes of the WFD, will only be useful where time dependent information on those groundwater bodies and associated surface water and terrestrial systems likely to be, or identified as being, at risk is also available.

Saturated and Unsaturated flow process representation.

Groundwater flow and contaminant transport modelling has, in general, evolved to deal with saturated flow conditions. The equations for flow and transport generally solved in distributed finite difference and finite element flow models and their associated contaminant tracking and transport codes only represent saturated flow conditions. The unsaturated zone is only taken into account as an integrated element in the recharge parameter. Calculations of the percentage of rainfall which recharges the saturated zone will include consideration of the characteristics of the unsaturated overburden. Under Irish conditions, this lack of specific modelling of flow and transport in the unsaturated zone is not necessarily a problem, owing to high precipitation rates the saturated zone is frequently at, or very close to, the ground surface. Also, thick sequences of (unsaturated) overburden are rare in Ireland, in comparison to, for example, America, and bedrock tends to be close to the surface. In addition, apart from sand and gravel, most Irish aquifers are fractured and are characterised by flow in fissures. This situation is reflected in the conservative approach to pollutant attenuation by the unsaturated zone adopted by the Geological Survey in assessing the vulnerability of bedrock aquifers: it is assumed that very little attenuation of pollutants will occur in unsaturated bedrock in which the flow is almost entirely by fissures (Misstear *et al*., 1999). Judgement should be used in assessing whether unsaturated flow is a large component of the system to be modelled.

Models of nutrient transport and distribution which involve processes in the root zone and subsoil will include a treatment of saturated-unsaturated flow .Network modelling of karst systems where conduit flow predominates, also assumes that there is no unsaturated flow. In cases appropriately represented by this type of model, with surface flow predominantly routing very rapidly via discrete fissures to groundwater, this assumption is valid.

The network models for contaminant transport, LandSim and ConSim, do include the capability to model unsaturated flow, either using a water balance approach or Richards equation for unsaturated flow. A small number of the most recently developed distributed models also include representation of unsaturated-saturated flow processes**.**

5.10. Type of model

Types of groundwater models relevant to implementation of the WFD in Ireland fall into the following three main categories a) Mass Balance Models b) Distributed Models and c) Network Models.

Mass Balance Models

Water balance models are based conservation of mass such that: Outflow – inflow = change in storage. The equation can be used to estimate missing information on variables. An example of a water balance equation to estimate recharge to an aquifer is:

Groundwater recharge = (precipitation + surface - water inflow + imported water + groundwater inflow) - (evapotranspiration + reservoir evaporation + surface water outflow + exported water + groundwater outflow) ± changes in surface water storage.

A water balance (or water budget) should form part of all groundwater modelling, to provide initial estimations of inputs, outputs and storage. A water balance can be calculated for either steady state or transient conditions. Water budget simulations should be compared with field estimated water balance to check accuracy and identify errors in model design- e.g. errors in transmissivity or storage estimations, or an invalid conceptual model. Estimation of errors in field data, should be included in the process.

Distributed Models (finite difference and finite element)

Distributed models solve the Darcian governing equation for saturated flow in two or three dimensions by numerical approximation across a discretised grid.

Numerical Approximations in Distributed models

For simple representations of flow, e.g. around wells, the governing equations can be simplified by e.g. assuming one- or two-dimensional flow and homogeneity of the medium, and solved analytically.

For more complex problems, the full mathematical model of a groundwater scenario is formed by a set of partial differential equations (the governing equations), boundary conditions and initial conditions. A computer code solves the set of algebraic equations generated by approximating the partial differential equations. The mostly commonly used numerical approximations of equations in groundwater are finite difference and finite element methods. A similar approach is used for surface water distributed models.

The continuous problem domain, (the area to be modelled) is replaced by a model domain discretised in both horizontal and vertical directions, and the model is described as a distributed model. The domain is represented by an array of nodes and their associated finite difference blocks or finite elements, forming a grid (finite difference) or mesh (finite element). The algebraic equations generated by the finite difference or finite element method are solved across the nodes of the grid or mesh. The number of dimensions that will be represented by the model and the level of detail required to achieve the desired result will inform the scale of discretisation of the grid in the vertical and horizontal directions. In groundwater studies, finite difference models have become the most generally used in research and industry. There are specific advantages relating to finite element models, but these are accompanied by higher skill and data requirements. It is not envisaged that the complexity of result which a finite element model can generate would generally be warranted in WFD implementation. The information below, therefore, focuses on the use of finite difference distributed models.

Number of Dimensions to be modelled in distributed models

Three-dimensional modelling has large data and processing time requirements. The practical solution to reduce the modelled dimensions from three to two, is appropriate only where this adequately represents the dominant characteristics of the hydrogeological system.

Most commonly used are two-dimensional areal models, that model vertically simple hydrogeological systems. They can be used to simulate a system where there is only one aquifer of importance, and can be confined, leaky confined, unconfined or varied spatially from confined to unconfined. Vertical flow through confining beds in the case of leaky confined aquifers is represented by a leakage term as described in the Darcian governing equation. These models can be used to model continuous porous media or fractured media using the EPM approach. There is an assumption of horizontal flow in both confined and unconfined aquifers. This assumption is true where the horizontal dimensions of the aquifer system are large in comparison with the vertical scale, (i.e. its thickness). Systems which requires detailed description of the hydraulic head distribution of an unconfined aquifer, such as with the modelling of a fen, where the ecosystem is dependant on micro-scale changes in groundwater level, are not suitable for modelling in two dimensions. In this case, the assumption of horizontal flow in modelling the unconfined aquifer is unfounded. Two dimensional models can, however, also be used at a smaller scale, where only the gross features of the system are required to be modelled, even if some of the characteristics of the system are not perfectly represented and where a degree of uncertainty regarding the fine detail of the model output is acceptable. This approach could be used in the identification of flow directions and the identification of linkages with surface water and wetland systems. Systems with large scale discrete fractures, e.g. karst, which under certain circumstances will be modelled using conduit flow models (see Network modelling of fractured media under conduit flow conditions below), can also be modelled, as an EPM order to ascertain regional flow gradients and associated flow directions. In this instance the modelled distribution of heads do not represent the true distribution, since the distribution is in reality associated with a network of discrete fractures.

Three-dimensional models can accurately simulate more complex hydrogeological systems than two-dimensional models. Vertical sequences of confined, unconfined, leaky confined and aquifers that vary spatially from confined to unconfined can be simulated. These models can be used to model continuous porous media or using the EPM approach. Full three dimensional governing equation allows for flow in all three dimensions, allowing the calculation of the three dimensional distribution of hydraulic heads in each layer. They can therefore be used to model confined and, in particular, unconfined flow where vertical flow gradients are important. In these models, the water table (and seepage face, if present) form part of the model boundary, and this can move in response to changing model stresses. Both finite difference and finite element models are able to simulate aquifers in profile, but movement of the water table and seepage face is handled more easily with a finite element model (Anderson and Woessner, 1992). The most widely used flow models and associated contaminant tracking and transport models are finite difference models.

Model outputs generally include a water balance and a distribution of hydraulic heads in each of the model layers, which can be viewed in a number of different ways; e.g. drawdown and equipotential lines. Three dimensional models are most useful when a detailed understanding of a hydrogeological flow system is required, in terms of hydraulic head distribution and gradient, resulting flow directions, magnitude of flux and, therefore, linkages with surface water bodies and associated terrestrial ecosystems.

A three dimensional model, that allows a surface water body to be modelled as a varying head boundary, is probably the only way to model the response of a surface water body to changes in the groundwater system to which the surface water body is hydrodynamically linked.

There are also some quasi three-dimensional models. These simulate a sequence of aquifers with intervening confining layers. The confining layers are not modelled explicitly and heads are not calculated for them, but their effect is simulated by a leakage term representing vertical flow between two aquifers. Since the confining layers are not explicitly modelled, a full data array is not required for each one, thus reducing the data requirements.

Data Requirements for distributed flow models

The generalised data requirements for a flow model fall into two broad categories: information on the physical framework (Table 5.2) and information on the hydrogeological framework (Box.5.1). These data together help formulate the conceptual model, construct model geometry and are used for calibration

Table 5.2. Physical Framework Data:

Physical framework, information mostly provided as maps and cross-sections:
Geological information on the areal and vertical extent and the boundaries of the system; Geological information on the extent, geometry, boundary elevations and thickness of aquifers and confining beds; Information on the extent and thickness of stream and lake sediments; Topographic data; Location and elevation of surface water bodies and divides.

Box 5.1. Hydrogeological Framework Data:

1) *Head and flux data consisting of:*
   Water table and potentiometric maps for each aquifer;
   Hydrographs of groundwater head and surface water levels and discharge rates.

2) *Aquifer Parameters consisting of:*
   Spatial Distribution of Hydraulic conductivity (K) and /or Transmissivity values for aquifers and confining beds. Vertically averaged (transmissivity) values will be required for 2-D areal modelling whereas a distribution of point measurements will be required for full there dimensional models. When simulating anisotropic media, information will be required on the three principle components of the hydraulic conductivity tensor, Kx, Ky,and Kz, though in practice vertical anisotropy is often unknown and estimated during calibration.Hydraulic conductivity values for and distribution for lake and river sediments; Storage properties of aquifer and confining beds if a transient simulation is to be run; Distribution of effective porosity values (for calculating average linear velocity) if particle tracking is to be carried out. Aquifer parameters are difficult to measure and therefore subject to uncertainty. Hydraulic conductivity ranges over 13 orders or magnitude and therefore potentially carries larger uncertainty than storage parameters and effective porosity which vary mainly within 1 order of magnitude.

3) *Aquifer Stresses:*
   Spatial (and temporal for transient simulations) distribution of recharge, evapotranspiration, natural groundwater discharge and groundwater pumping rates.

Model boundaries will be defined from the data above. Boundary conditions are mathematical statements specifying the dependant variable (hydraulic head) or its derivative flux at the boundaries of the problem domain. Boundaries are either physical or hydraulic and consist of specified head and specified flux boundaries, including constant head and flux, and head-dependant flow boundaries. These boundary types can be assigned as external model boundaries at the model extents and as internal boundaries where they represent features within the modelled area, for example lakes or rivers.

Parameter values assigned to the model grid or mesh, which represents the hydrogeological system to be modelled, form the initial conditions for the modelling process.

Particle tracking for flow system analysis and pollutant transport in distributed models

Particle tracking is used to trace outflow paths or pathlines, by tracking the movement of infinitesimally small imaginary particles placed in a flow field. It is carried out after running a continuous porous medium or EPM flow model, which generates a head distribution, which is used to calculate a velocity distribution, which is then used to trace out pathlines. Particles can be tracked from the results of two- and three-dimensional, steady-state and transient simulations. The number of dimensions of the flow model supplying the data and the chosen tracking code determine the number of dimensions in which the particles will be tracked.

Particle tracking assumes that a particle moves by advection at the average linear velocity of groundwater (v). In numerical particle tracking codes, the particles introduced into the flow field move in a continuous spatial domain according to the velocity distribution calculated from the head distribution. The velocities are calculated from a head distribution known only at discrete points, and interpolation is required to calculate velocities at particle locations. A particle tracking scheme that tracks particles along pathlines is solved in the full three-dimensional case:

$$dx/dt = v_x$$
$$dy/dt = v_y$$
$$dz/dt = v_z$$

according to one of four commonly used integration methods.

Particle tracking is a useful tool in the analysis of flow in the groundwater system. Particles placed around the perimeter of the model will yield a picture of the flow field. Areas of recharge and discharge, with their associated flow paths at a variety of scales, local to regional, can be determined.

Transport of contaminants is affected by advection, dispersion and chemical reactions. Particle tracking can be used in certain situations as a simplified alternative to solving the full advection dispersion equation, in order to estimate and average time to discharge

Reverse particle tracking allows the introduction of particles at a chosen location (well, surface water body, wetland or site) at which contamination is detected. The particles are then virtually tracked back along modelled pathlines to their source. This can be used in the delineation of well capture zones, for the purposes of well head protection or the identification of linkages between groundwater recharge and surface water bodies or wetlands. Time related capture zones can also be calculated.

Full (Distributed) Pollutant Transport Modelling

Full description of the transport of a contaminant solute involves consideration not just of advection (above) but also dispersion and chemical reactions. As with particle tracking, full solute transport modelling for distributed models is based on the head distribution results from a distributed flow model, from which an average linear velocity field is calculated.

The governing advection dispersion equation for solute transport, is difficult to solve, and both finite difference and finite element solutions are affected by numerical errors. Assigning appropriate grid and time step spacing is critical in reducing these errors. In order to reduce the problems associated with finite difference and finite element solutions, some codes use particle tracking methods to solve the advection portion of the equation, combined with some other method, such as finite difference for the other portions. Use of a full solute transport model is necessary when temporal and spatial concentration of a contaminant is required. The processes modelled, in addition to advection, affect solute transport simulations. The result must be qualified by an understanding of the uncertainties inherent in this type of modelling.

There are also some particle tracking codes which solve the dispersion portion of the governing equation. Where it is likely that advection and dispersion are the dominant processes affecting transport of contaminants, such a model can decrease uncertainty associated with the other elements of the dispersion-advection equation.

Multiphase flow

The transport equations described above apply to miscible fluids. Multiphase flow refers to the movement of water and one or more immiscible phases, also known as non-aqueous phase liquids (NAPLs). The governing equations for multiphase flow are different and are formulated in terms of the pressure of each of the phases. Modelling of NAPLs is unlikely to be required frequently under the WFD, as it is usually associated with localised contaminated land sites. Where a model listed below supports simulation of multiphase flow it is included in the model description.

Density dependant flow of Miscible Fluids

Density dependant flow includes salt water intrusion. A requirement for identification of risks from saline intrusion is included in the WFD. It is not considered to be a significant pressure under Irish conditions. The only areas at risk may be islands or coastal areas where there is natural intrusion. It is considered that appropriate engineering and management of groundwater supply boreholes will avoid any risk of supply contamination or increased intrusion. Data requirements for distributed full transport modelling vary with the processes being simulated and the number of dimensions being represented.

Availability and Choice of validated Flow, Particle Tracking and Solute Transport and Modelling software:

Choice of Modelling Software

Distributed flow and distributed contaminant modelling codes may perform a single task or more that one task. For example, two dimensional flow modelling, particle tracking and solute transport all the in the one code.

Commercially available modelling codes generally consist of a combination of an original modelling code, frequently the result of a research project, or the product of some interested organisation, which may itself be available as freeware e.g. USGS MODFLOW, and pre- and post-processors designed by a commercial company. Commercially available codes are also sold in software suites of related models, essentially modelling environments, for example, a three-dimensional flow model, a calibration code, a three dimensional particle tracking code and a three dimensional solute transport code, with pre-and post-processors. The pre-processor usually consist of an interface designed to facilitate easy data input, running of, and seamless transfer of data between, the models, with post processing graphical capabilities for displaying results. Many of the modelling codes which have become industry standards are available from the original developers (e.g. US EPA and USGS) as freeware. Pre- and post- processors and other related software are also available, although the interfaces may not be as user friendly as commercially developed ones.

There is such a profusion of interrelated models, many of them developed from the same original code, that only short descriptions are included in this chapter. The models discussed here are only a number of the possible available models. They have been chosen as having been well validated through use in industry and research or new versions of existing validated models, but with additional features which make them useful tools to help with the implementation of the WFD. Longer descriptions of a single example of each of 2D, 3-D and pollutant transport models are included in Annex 1.

The choice of modelling software or modelling software suite will depend on the model codes(s) required to carry out modelling appropriate to the groundwater system and achieve the result required. The decision will also include the cost of commercially available products, the ease of use of the pre-and post processors, what additional useful tools are provided as part of a suite of modelling software, and familiarity with a given code or software**.**

Commonly used software for distributed flow modelling:

Two-dimensional Flow and Particle tracking models

Flowpath II. A two dimensional (2-D) areal, finite difference, groundwater flow, pathline (particle tracking) and contaminant modelling package.
Developed by and commercially available from Waterloo Hydrogeological http://www.flowpath.com.

WHPA. 2-D areal semi-analytical flow and particle tracking model consisting of four modules designed for delineating capture zones in a wellhead protection area. There is some quantification of the effects of uncertain input parameters. Developed by and available as free-ware from the U.S. E.P.A. http://www.epa.gov/ada/csmos/models.

MODFE Vers. 1.2. 2-D modular finite element flow model for areal and axisymmetric problems. It allows the simulation of leaky, confined and unconfined aquifers of anisotropic and heterogenous porous media. Both steady-state and transient conditions can be simulated. There is no probabilistic modelling capability.Developed by and available as freeware from the U.S. Geological Survey (USGS) at http://water.usgs.gov/nrp/gwsoftware/.

3-Dimensional Flow models

MODFLOW 3-D finite difference flow code has become the industry standard in 3-D modelling software. It was originally developed by the US geological Survey (USGS). Current versions from the USGS are MODFLOW-2000 and MODFLOW-GWT.. The USGS has developed associated particle tracking and contaminant transport models, as well as other supporting modelling tools and input and display pre-and post-processors. Other organisations and commercial companies have developed particle tracking and contaminant transport models which take their input flow data from MODFLOW, as well as tools and pre- and post-processors.

The USGS website also includes numerous practical reports on using their codes, manuals and references. Developed by and available as freeware from the USGS at http://water.usgs.gov/nrp/gwsoftware/.

MODFLOW-SURFACT Version of MODFLOW, developed to address some of the limitations of MODFLOW and including transport modelling capabilities. The MODFLOW-SURFACT Transport (Advanced) includes unsaturated zone flow modelling capabilities, dual porosity and fracture zone modelling and improves modelling of the dynamic saturated/unsaturated interface. As well as multi-contaminant solute transport it includes simulation of multi-phase transport and dissolution and volatilisation of NAPLs. The software is not capable of producing a probabilistic result. It is also integrated into Waterloo Hydrogeologic's Visual MODFLOW suite, Developed by and available from HydroGeoLogic Inc. http://www.hgl.com/ and Waterloo Hydrogeologic at http://www.flowpath.com.

FEFLOW3D 3-D finite element flow and solute transport model for steady state and transient conditions. It is one of the most widely used FE models used in industry for complex modelling problems which warrant a finite element approach. It includes simulation of saturated and unsaturated flow, density dependant flow, and mass and heat transport. It includes 3-D visualisation tools, mesh generation and interpolation tools and an ARC/INFO GIS interface, and is available from Waterloo Hydrogeologic, http://www.flowpath.com/software/software_main.htm

3-Dimensional Particle Tracking

MODPATH Particle tracking postprocessing package developed to compute tree-dimensional flow paths using output from steady-state or transient groundwater flow simulations by MODFLOW. It uses as a semi-analytical particle tracking scheme.
MODPATH Developed by and available as freeware from the USGS at http://water.usgs.gov/nrp/gwsoftware/.

3-Dimensional Transport Models

MOC3D Three-dimensional ground water flow and solute transport for both steady state and transient conditions. The transport model is integrated with MODFLOW. MOC3D uses the method-of-characteristics to solve the transport equation. The model was developed by, and available as freeware, from the USGS at http://water.usgs.gov/nrp/gwsoftware/.

MT3D99 Three-dimensional numerical model for simulating solute transport in complex hydrogeologic settings, using flow data from finite difference models.
Developed by and available from S.S. Papadopulos & Associates, Inc. at http://www.sspa.com/products.

HST3D 3-D finite element model which simulates ground-water flow and associated heat and solute transport in three dimensions. Variable density fluids can be modelled.Developed by and available as freeware from the USGS at http://water.usgs.gov/nrp/gwsoftware/.

Multi-phase Flow Modelling

MODFLOW-SURFACT (see above)

The US EPA have developed various models with very specific contaminant and NAPL modelling capabilities. These include models that are applicable to transport and attenuation of specific contaminants in particular conditions. Available at http://www.epa.gov/ada/csmos.

Density dependent Flow Modelling

SUTRA 2-D finite element model for saturated-unsaturated, fluid density-dependent flow of solute or energy, for steady-state or transient conditions. Developed by and available from the USGS at http://water.usgs.gov/nrp/gwsoftware/.

MOCDENSE 2D method of characteristics, 2-constituent, solute-transport model for variable density ground water. Developed by and available from the USGS at http://water.usgs.gov/nrp/gwsoftware/.

FEFLOW3D (see description above)

Commercial suites of flow and transport modelling software

Commercial suites of software in a modelling environment include and support similar models. Some will include and support more or different models to another. Their display capabilities may be different or they may require additional software for display, and some support probabilistic modelling and exchange with GIS software. Choice of suite will depend on what is required by the user at the time and in the future.

Examples include:

- Groundwater Vistas, developed by and available from Environmental Simulations Limited at http://www.groundwatermodels.com.
- Processing Modflow PRO available from Integrated Environmental Services, Inc. at http://www.iesinet.com/products
- Visual MODFLOW Pro 3.1 developed by and available from Waterloo Hydrogeologic at http://www.flowpath.com/

Modelling Support Tools

Other programmes related to and which facilitate the modelling process include:

- SURFER Vers. 8 Data processing and interpolation tool, with a number of interpolation techniques, contouring and extensive grid preparation tools. Developed by and available from Golden Software Inc. at http://www.goldensoftware.com

- Visual PEST-ASP Model independent, parameter estimation programme which uses a numerical inverse-problem solver. It is a very powerful tool, which can be used with almost any type of model.Developed by WaterMark Numerical Computing at http://www.ozemail.com.au/~wcomp, suppliers include Environmental Simulations Limited at
- http://www.groundwatermodels.com

- MODTOOLS (GIS) Set of computer programs for translating data of the ground-water flow model, MODFLOW, and the particle-tracker, MODPATH, into a Geographic Information System (GIS). These tools can also be used to take the generic MODFLOW and MODPATH result files from any of the commercial modelling suites e.g. Groundwater Vistas. Developed by and available from USGS at http://water.usgs.gov/nrp/gwsoftware/.

Network Models

Network Models for contaminant transport

There are a number of network type models which have been developed specifically for site specific assessment of risk to ground and surface waters posed by point source contamination. These models are risk assessment tools. A point source, pathway and receptor are identified and in some of the models multiple sources and receptors in, and pathways through, the one hydrogeological system can be modelled. The models link the source node, to nodes in each of the hydrogeological units which comprise the pathway, to the receptor node. The complexity of models vary.

These models are designed to simulate contaminant transport in porous media having continuous interconnected pore space, or for media which can be modelled as EPMs. Darcy’s law and Richards equations are used for flow and the contaminant transport equations for advection, dispersion, retardation and decay outlined above are solved.

The commercial models referred to below are capable of being run in probabilistic mode, using a Monte Carlo simulation. Various parameters including hydraulic conductivity and contaminant concentration can be chosen as the random variable to be used in the Monte Carlo simulation. This allows a full probabilistic risk assessment to be achieved.

A risk assessment conceptual model must be developed in conjunction with the hydrogeological conceptual model. Unlike a finite difference or element based distributed contaminant model these models do not take input directly from a flow model. Information from hydrogeological investigations or from some appropriate flow model are needed. Information on sources, contaminants involved, the hydrogeology of the units comprising the system (including flow gradients and fluxes), the geometry of the pathways and the attenuation processes to be modelled along the pathways must all be provided the user.

Such network models are essentially one or two-dimensional. With the commercially available and validated model RAM the result is only reported at the receptor(s), with LandSim both lateral and longitudinal dispersion is taken into account and it is possible to view the concentration along the contaminant plume in plan view.

The commercial models referred below are designed to deal with miscible liquids, and make no special provision for modelling imiscible liquids (NAPLs).

Data Requirements for Network Models for contaminant transport

The level of data required for the model will vary according to the complexity of the geometry of the network model and on the and type of processes being modelled along the pathways. For each additional source, pathway, receptor in the network, information for the source, each hydrogeological unit in the pathway and the receptor will be required at the level demanded by the process being modelled. For probabilistic results, information on the distribution of the parameter to be used as the random variable for the simulation must be provided.

A simple network of a landfill source with no processes, a one (aquifer) hydrogeological unit pathway with dilution, to a receptor in that unit could require: Source geometry, water balance and contaminant concentration; Contaminant properties and receptor standard for the contaminant; pathway hydrogeological unit water balance, hydraulic conductivity (K), hydraulic gradient (i) and geometry; Any additional receptor dilution;

An assessment for the same simple network structure, where advection, dispersion, retardation and decay processes are modelled in the aquifer pathway unit could require, in addition to the above:

Decay rate constant, diffusion co-efficient and partition coefficient for each contaminants being modelled; Porosity, dry bulk density and tortuosity of the pathway unit; Travel distance from the source to the receptor within the unit.

Validated Network Models for contaminant transport

RAM is an example of a general point source contaminant transport modelling software. It is a risk assessment based model which allows the prediction of contaminant transport and fate. Developed by and available from Environmental Simulations International at http://www.groundwatermodels.com/.

LandSim 2 and ConSim 2 are very similar in structure and data requirements to RAM but are more specialised in their application. LandSim has been specifically designed to deal with landfill contamination, and ConSim to deal with contaminated land sites. However, they allow only multiple source landfill or contaminated land sites, but not multiple pathway or receptor networks. They do however include a capability for modelling the engineered structures of the site e.g. landfill liners. Both were developed on behalf of the British EA.Developed by and are available from Golder Associates, see www.landsim.co.uk and www.consim.co.uk

Network Modelling of fractured media under conduit flow conditions

Where a fractured medium has very large, discrete fractures in which conduit flow is occurring and the scale of the groundwater system to be modelled is too large (i.e. the area under consideration too small) for equivalent hydraulic properties to be defined from a REV, the EPM approach is probably not appropriate. Under Irish conditions, this is most likely to occur in karstifed limestone. In karst both primary and secondary porosity can be enlarged over time, creating a system of pathways of high hydraulic conductivity. Where the limestone is heavily karstified, conduit flow can predominate and distributed flow form only a minor component of the overall flow. Such systems are characterised by drainage via discrete pathways for underground water. The hydrogeological regime cannot be neatly divided into the traditional ground and surface water components, and any modelling approach must integrate both components. The system cannot be represented using EPM modelling, since this would mask the effect of the discrete pathways of much of the subsurface flow, which component is, in addition, not moving under Darcian flow principles.

Choice of modelling approach in karstified areas

Possible approaches which take into account the characteristics of heavily karstified fractured systems and their requirements in terms of integrated modelling include a linear systems approach, pipe representation of karstic flows and network modelling.

A linear systems approach involves deriving a function to relate rainfall input to a point output (discharge), such as at a karstic spring. The model is a lumped one and interpretation of flows and levels at intermediate locations is difficult. This approach would not be suitable where information on levels and flows at individual locations across a region are required. Where there is little data and the information required is at a small scale (regional level), or where only basic flow information is required, a black box model may be appropriate. Springflow is frequently used to represent the response of the groundwater to recharge or stress.

Pipe network representation of karstic flows has been undertaken, but require very detailed knowledge of the geometry of the pipes and the approach is therefore not readily utilized in regional systems.

Network modelling represents an intermediate approach, where flow routes can be modelled discretely, represented by a series of links and nodes, allowing simulation of level and flow at points across a regional system, but not requiring detailed information for each conduit. Conduit flow models require a very good understanding of the topology and connectivity of the flow system, and as such are very data intensive. Measuring the flow characteristics of the system is difficult and time consuming. Examples of where it may be appropriate include:

- Local (large scale models) where flow to an important groundwater dependant ecosystem is dominated by conduit flow, for example some turloughs; and
- Large scale models for source protection, where well recharge is dominated by conduit flow or the source is a spring.

Validated Network Model for Irish Karst

A network modelling approach has been validated for Irish karst conditions in the Gort lowlands, using the HYDROWORKS commercial sewer pipe modelling software (Johnston and Peach, 2000). Although the HYDROWORKS model has been extensively validated for modelling sewer networks this appears to be the first time that such a model has been applied to a complex regional karst system. This application was very successful. A description of software is not included in the templates since this is a specialised, non-standard application of the model.

The objectives of the modelling included gaining an understanding of the hydrodynamic regime within the turloughs in the system, the ecosystems that they support being proposed for protection as SACs [under the Habitats Directive]. The model was validated using a second data set and there was good agreement between observed and predicted values.

A network model consists of nodes and links. In modelling karst, the conceptual model becomes one of a network of conduit links connected by nodal storages. The links can represent a single conduit, or an active fracture system acting under a pressure head. Detailed geometry of the link is not required. Nodes in the network need to be able to represent meeting points of conduits, closed and open water storages, the latter in order to represent lakes and turloughs, and must accept input coming from surface water flows and from recharge from net rainfall. The model requires water level information at the outlet of the network.

The application of a network model requires an understanding of the topology and geometry of the network nodes and links. This is derived from a strong understanding of the karst hydrology and genesis and used to define the geometry and topology of the network. The properties of the links are determined by calibration and adjustment to achieve observed hydraulic responses. This requires that data for calibration is available across the area of the model.

Inflow to the model comes from recharge from net rainfall and from surface water flows. Each of these inflow components is modelled separately. In the Irish application referred to above, the IHACRES rainfall-runoff model was used to simulate integrated catchment runoff to provide suitable surface water flow inputs to the model. Direct rainfall recharge to the network model was calculated in a Geographical Information System (GIS) environment on a grid square basis. Inflows are then assigned to selected network nodes. The accuracy of a network model result is highly dependent on the ability to model the inflows accurately.

This model can be run in transient mode, where time series data is available for inflows and outflows. Outputs are water levels and flow rates in the different elements of the system over time.

5.11. Availability of Data, Interpolation and Estimation of Parameters by Calibration

The type and scale of model that can be used is highly dependent on the availability of appropriate data. The amount of data required for a model will generally increase with***:***

- Complexity of the hydrogeological system to be modelled;
- Level of detail of the result required;
- Number of dimensions to be modelled;
- Modelling of transient rather than steady –state conditions
- Probabilistic compared with Deterministic simulation

Data Availability

Collection of hydrogeological data is difficult. In Ireland there is a lack of groundwater head and flux data and general hydrogeological information. Not withstanding the efforts of the Geological Survey in collecting existing data, and the more recent efforts of the EPA, there has been, and still is, no programme of monitoring of boreholes specifically for the purposes of groundwater data collection. Only existing hydrogeological data will be available for the initial characterisation phase required under Article 5 of the WFD. Additional data will come on line as *surveillance monitoring* and later *operational* monitoring proceed according to the requirements of Article 8. Modelling carried out during the initial characterisation phase, and any existing or new vulnerability assessment should aid in identifying lack of data and in optimising monitoring programmes to collect data required for the further characterisation stage. Surveillance monitoring and subsequent operational monitoring will aid, and should be responsive to the needs of, groundwater modelling.

Interpolation

For distributed flow models, parameter values must be assigned to each node, cell or element of a model grid. In the absence of sufficient field data, interpolation of measured data points can be carried out to estimate the spatial variability of values across the model domain. Statistical interpolation methods include kriging, triangulation, polynomial regression and inverse distance methods. Parameter values may also be assigned using hydrogeologic judgement. Of the statistical methods kriging is extensively used, because it considers the spatial structure of the variable, taking into account distance to the field measured points and also preserves them in the result. Disaggregation of data can also be carried out but only where it is known that the spatial or temporal variability of the data is low.

Parameter Estimation by Calibration

Initial model parameters and boundaries essentially become variables during the calibration process. After the initial model run, the parameters and boundary conditions are modified in order to improve the fit of the model to field observed data. Ideally there should be sufficient head and flux data to model using a split data set, where one set of data is used to calibrate the model and the second is used to compare with the calibration result to validate it, though this is frequently not the case. Altering the parameters and boundary conditions to improve fit is a solution of the inverse problem, that is, estimating model parameters and gaining increasing information about the model domain characteristics and flow mechanisms through the model process. Estimation of the model parameters can either be carried out subjectively using expert knowledge, by ‘trial and error’ calibration or by objective mathematically constrained optimisation methods.

5.12. Identifying uncertainty in the modelling process.

The accuracy of model output is dependent on several factors:

- Representation of processes. The degree of uncertainty will relate to the extent to which actual physical and chemical processes are represented in the model. The processes that can be modelled using Darcian equations are well understood, however the processes involved in fracture flow are less well understood, and the reliability of the equations used to represent them lower, introducing a high level of uncertainty in the model results. In the case of contaminant transport, there are still unresolved problems in developing dispersion and chemical reaction theories that apply to field problems. Only the advection element of contaminant transport is well understood and, therefore, reliably represented in groundwater models. This introduces a high level of uncertainty into the results of currently available solute transport codes applied to complex contaminant scenarios. In the case of groundwater interactions with surface waters, and saturated - unsaturated zone interactions, which require representation in nutrient modelling, there is a lack of understanding of some of the processes involved, at both large and small scales. More general examples of processes that are often ignored or represented only in an approximate way, include, the three-dimensional pattern of flow in almost all aquifers and horizontal and vertical variability of flows in most aquifers.

- Numerical Methods.
  Numerical solutions of equations chosen to represent systems are subject to errors.

- Lack of, or errors in input data and parameter interpolation.

Model choice and implementation should aim to minimise these sources of uncertainty. Existing sources of uncertainty should at least be identified and taken into account in interpreting model results. Sensitivity analysis should be, but is not in practise, generally carried out.

Where uncertainty in a parameter can be identified and measured, this information can be used to generate probabilistic output from a model. Where a parameter with a measured uncertain distribution is used as input, a probable result can be generated. This probabilistic output can provide the probability of occurrence element of a risk assessment.

5.13. Level of validation of model

Owing to the short time scale available for initial implementation of the River Basin Management Plans, at least for the first implementation, there will not be time for the development of new computerised codes for numerical modelling, or their verification. Consequently, only equations which are represented analytically or numerically in existing software codes, which have already been extensively used either in Ireland or abroad and considered to be sufficiently validated in the course of this use, will be available for representing and quantifying groundwater processes. All of the models referred to in this section are considered to fall into this category of sufficiently validated models.

5.14. Interface of models with Geographical Information System (GIS) data

Gridded GIS data is structurally similar to that input to, and resulting from, distributed finite difference and finite element flow and transport codes. Several such modelling codes have pre- and post-processors which interface easily with GIS data. Some of the data available for implementation of the WFD is available in GIS This is useful for decreasing the effort in constructing gridded data for input to flow models and also for analysis of spatial co-incidence of pressures and potential at risk ground and surface water bodies. It may also provide an exchange or integrating format between ground and surface water models. In addition there is a requirement for spatial information recorded during River Basin District Management Plans to be available in GIS format. Distributed finite difference and finite element model results can relatively easily be translated into GIS grid data. See also discussion on application of GIS to implementation of the WFD in Chapter 2.

Issues signalled in *Model Choice* above should be addressed in choosing an appropriate approach to the specific hydrogeological/hydrological task.

5.15. Initial Characterisation

Potential roles for modelling in the delineation of groundwater bodies and their initial characterisation include:

- Use of any existing groundwater and solute transport models to provide information about the flow system characteristics and parameters, and any modelled pollutant location or distribution. Flow system characteristics which can be modelled include: Groundwater hydraulic head, which can be described as groundwater level, and which in the context of the directive, is taken as the key indicator of quantity; Flow type, direction, distribution and flux, as well as linkages with associated surface water bodies and terrestrial ecosystems.

- Water balance modelling. Water balance calculations can be used to give an initial estimate of amount and location of recharge, discharge from and storage in the system, this information will aid in development of a conceptual model of the system.

- Development of 2-dimensional distributed flow models, where an Equivalent Porous Medium approach is appropriate. Modelling would be carried out in an evaluation role, using the calibration process to gain information about model parameters and boundary conditions about which there is little information. Such models can provide an overview of flow characteristics and parameters in the hydrogeological system, taking into account the uncertainty associated with the assumption of horizontal flow in 2-dimensional models. Flow paths estimated from particle tracking, using the flow model results, could be used to identify areas of recharge and discharge to the groundwater body and indicate linkages with dependant surface water bodies and ground water dependant terrestrial ecosystems.

5.16. Further Characterisation

Indicative approaches to the process of further characterisation, to be carried out in the context of, and integrated with, the modelling required for estimation of risk are outlined below.

Modelling for characterisation of head distributions, fluxes and flow paths within the water body and for characterisation of fluxes and heads in linked associated surface water and terrestrial systems could include:

- 2- D distributed modelling in evaluation mode for simple regional and local hydrogeological systems, which can be represented as an EPM, where flow is adequately described by two dimensional representation and vertical flow gradients are not significant. Associated particle tracking. e.g. FlowPath II
- 3-Dimensional distributed modelling in evaluation mode, for more complex systems, generally local, which can be represented as an EPM and where a detailed distribution of heads and fluxes are required to characterise the system and linkages with surface water and terrestrial ecosystems. Associated particle tracking. e.g. MODFLOW, MODPATH
- Network modelling of conduit flow, in evaluation mode, for karst systems where conduit flow dominates. e.g. HYDROWORKS

5.17. Pressure State Modelling

Table 5.3. provides indicative approaches to pressure-state modelling in groundwaters. The modelling can be carried out in two possible modes:

- Evaluation mode, whereby the current *state* or characteristics of the ground water system with existing pressures is modelled, providing a measure of variables which impact on a given receptor. This allows identification of the current status of a receptor in comparison with the environmental objectives defined for that receptor.

- Predictive mode, where a calibrated model is run in a 'what if' scenario, to predict the response of the hydrological system to some pressure, that is, change in the system, for example dewatering at a quarry site, and to predicts the state at some receptor. Predictive modelling can also be used to assess the effectiveness of proposed measures or *response* in achieving environmental objectives for a receptor.

Table 5.3. Indicative table of modelling approaches to pressures applicable to groundwaters

Driver	Hazard	Pathway	Receptor(s)	Receptor characteristics at risk	Model approach	model purpose	Model e.gs.
Abstraction: e.g. Industrial including, quarry and mine dewatering, agriculture, Private and public water supply	changing water levels	internal	local g/water body local d.w. abstraction	Quantity, therefore Quality	2-D, 3-D distributed F.D. or F.E.,, particle tracking, Network conduit	Evaluation or prediction	WHEPA, FLOWPATH MODPATH MODFE HYDROWORKS
		external	s/w quality standards local s/water ecological system local terrestrial ecosystem	Quantity, therefore Quality	2-D, 3-D distributed F.D. or F.E., particle tracking, Network conduit	Evaluation or prediction	WHEPA, FLOWPATH MODFLOW MODPATH MODFE, HYDROWORKS
Landfill	leachate pollutant, priority substances	internal	g/water body d.w. abstraction	Quality	Network contaminant, 2-D, 3-D distributed with part tracking and contam transport	Evaluation or prediction	RAM LandSim, FLOWPATH MODFLOW MT3D FEFLOW3D
		external	s/w quality standards s/water ecological system terrestrial ecosystem	Quality	Network contaminant, 2-D, 3-D distributed with part tracking and contam transport	Evaluation or prediction	RAM, LandSim, FLOWPATH MODFLOW MT3D FEFLOW3D

Table 5.3. continued

Point source contamination: e.g. Decomissioned mine, mine tailing ponds,	pollutant, priority substances	internal	g/water body d.w. abstraction	Quality	Network contaminant, 2-D, 3-D distributed F.D, F.E with part tracking and contam transport	Evaluation or prediction	RAM FLOWPATH MODFLOW MT3D FEFLOW, MODFLOW-SURFACT
		external	s/w quality standards s/water ecological system terrestrial ecosystem	Quality	Network contaminant, 2-D, 3-D distributed with part tracking and contam transport	Evaluation or prediction	RAM, FLOWPATH MODFLOW MT3D FEFLOW MODFLOW-SURFACT
Salt water intrusion	saline water	internal	g/water body d.w. abstraction	Quality	Density dependant flow model	Evaluation or prediction	SUTRA, FEFLO3D
		external	s/water ecological system terrestrial ecosystem	Quality	Density dependant flow model	Evaluation or prediction	SUTRA, FEFLO3D

Table 5.3. continued

Historical contaminated land	pollutant priority substances NAPLS	internal	g/water body d.w. abstraction	Quality	Network contaminant, 2-D, 3-D distributed F.D, F.E with part tracking and contam transport, multi-phase flow models	Evaluation or prediction	RAM, FLOWPATH MODFLOW MT3D FEFLOW U.S. EPA models MODFLOW-SURFACT
		external	s/w quality standards s/water ecological system terrestrial ecosystem	Quality	Network contaminant, 2-D, 3-D distributed F.D, F.E with part tracking and contam transport, multi-phase flow models	Evaluation or prediction	RAM, FLOWPATH MODFLOW MT3D FEFLOW U.S. EPA models MODFLOW-SURFACT
Diffuse Source pollution from mainly Agriculture Septic tanks	Nitrogen and Phosphorus movement		Incidental, overland flow and preferential sub-surface flow	Quantity, therefore Quality	Network contaminant Multi-phase flow models	Evaluation or prediction	NCYCLE ANIMO NLEAP RZWQM

5.18. Modelling nutrient transport to groundwater

As with other branches of contaminant transport modelling in the hydrological cycle, the framework underlying most models of nutrient movement is one of 'source-pathway-receptor'. What often distinguishes the modelling of nitrogen and phosphorus in groundwater is that the pathway stops short of the ultimate surface water receptor demanded by the WFD. While the groundwater body itself may be the receptor in a model, it is the ecosystem into which the groundwater body discharges which may be at risk – e.g. in springs, wetlands, rivers and estuaries. This gap may necessitate a linking analysis (or a further model) between the output of a nutrient transport model and the receptor of concern. Nevertheless, groundwater, as a receptor in its own right, may require modelling for determining the status. Sometimes it is then the implied downgradient effects that determine the acceptable concentrations of N and P in the groundwater body. Such is the basis of the EU Nitrate Directive (91/676/EEC), the principles of which are subsumed into the WFD. The receptor may be defined as groundwater but with reference to downgradient impacts.

Like other groundwater models, nutrient transport models may only address the 'contaminant' in a generic fashion (i.e. 'intrinsic' modelling, treating the worst case of the contaminant travelling down the pathway at its maximum velocity, that of the groundwater drainage) or they may address the nutrient behaviour specifically. The former is the basis of the risk-based groundwater protection schemes applied in Ireland and which apply to nutrients as well as to any other 'generic' contaminant. The risk of unacceptable contamination in the aquifer is related directly to the thickness of the subsoil overburden and inversely related to the indexed hydraulic conductivity of the subsoil. The determined risk then also depends on the relative value or importance of the aquifer or groundwater body. Such models are, of necessity, blunt-edged instruments in relation to nutrient transport, but are proving of value in managing land use and potentially polluting activities. Indexed levels of each parameter can assist implementation through GIS/mapping.

Models of intrinsic transport have been developed widely for predicting nutrient and pesticide concentrations in groundwater bodies driven by needs such as the Nitrate

Directive and Drinking Water Directive. The focus has been on nitrates, phosphorus and on groups of herbicides and/or pesticides. The sources of nutrient contamination is often assumed to be agricultural practice, but sources such as septic tank and other wastewater discharges to soil may be significant. However, it is the problems sourcing from agriculture which have driven model development. P and particularly N may undergo significant biogeochemical transformation along the pathway between source and groundwater receptor. Thus, characterizing the source (or loading) is a key part of the modelling exercise. Although there are significant areas of arable farming in the southeast, agriculture in Ireland is dominated by grassland and animal husbandry which has particular implications for determining loading and the likely release of nutrients (leaching) into the subsurface pathways. Moreover, it has become widely recognized that the driving mechanisms for nutrient transport to groundwater is a combination of hydraulic (effective rainfall, irrigation, water content of slurries) and contaminant loading (i.e. N or P content).

Types of intrinsic nutrient transport model:

Nutrient (and pesticide) transport models for defining impact on groundwater can be classified into two broad categories:

- Loading models: these effectively define the source loading at the base of the root zone with the implication that that is related to the groundwater concentrations. They do not treat any of the physical processes in the rest of the unsaturated zone or in the groundwater itself, such as dispersion, dilution and adsorption; and
- Process models: these attempt to model the hydrochemical processes involved, both in the loading (root) zone as well as in the unsaturated soil-water zone and in the groundwater, saturated zone.

As with other modelling approaches, the more detailed the attempt at modelling the processes, the more data are required. The selection of model depends, as usual, on the objective and the exigencies of time and money. While most of the models described are not specifically probabilistic, most can be put into such a framework for the purposes of risk assessment through the use of procedures such as Monte Carlo simulation.

Loading models :

These might be described as mass balance models but the implication is that they deliver an output from the agricultural activity near the surface and in the root zone for delivery to the underlying 'groundwater' which may include unsaturated/saturated conditions.

A simple example for nitrogen is the Dutch mass balance model:

$$[NO_3] = \{(N_{sur}+N_{dip}+N_{fix}) - (N_{vol}+N_{den}+N_{run}+N_{imm})/V_{gw}\} \text{ x } F_{NO3} \text{ x } 62/14$$

where

NO_3 = "nitrate concentration in groundwater (mg/l)"

N_{sur} = calculated nitrate residual (kg/ha)

N_{dip} = nitrogen input from atmospheric deposition (kg/ha)

N_{fix} = nitrogen fixation from atmospheric N (kg/ha)

N_{vol} = nitrogen loss through volatalization (kg/ha)

N_{den} = nitrogen loss through denitrification (kg/ha)

N_{run} = nitrogen loss to runoff and land drainage (kg/ha)

N_{imm} = nitrogen storage in the soil (kg/ha)

V_{gw} = groundwater recharge (10^3 m^3 /ha/yr)

F_{NO3} = fraction of nitrate in nitrogen recharge

62/14 = conversion, nitrogen N to nitrate N

This equation is typical of many loading models and raises the common issue of the uncertainty in many of the parameters listed. Evaluation often rests on a combination of results from careful, site-based research work and empirical assessment. Other loading models are effectively characterized by their ability to better represent one or more of these terms. Examples of loading models which calculate N-input to the groundwater system, usually from the base of the root zone include NCYCLE (UK), see section 3.3.5., ANIMO (Netherlands), section 3.3.4. and NLEAP (USDA), and RZWQM (USDA).

Any of these models could be used (subject to their own limitations) for either a screening device for determining potential nutrient losses to groundwater or as an input to a separate groundwater transport model. They all incorporate measures of agricultural management and practice and are essentially one-dimensional in form.
Listed in order of increasing complexity, the more comprehensive models (e.g. RZWQM) attempt to represent the processes of transformation of N within the root zone in a more detailed way.

Process models :
Such models represent not only the biogeochemical transformation of the species, such as N or P, but also the transport dynamics to and within the saturated groundwater zone. As for other groundwater/mass transport models, the framework of model construction is primarily based on hydrological modelling upon which the transport model is grafted. Primarily, the hydrological model for unsaturated transport is the Richard's equation and for saturated flow, the advection- dispersion equation. They are both based on Darcy's law for flow in porous media but the Richard's equation depends on knowing the relationship between hydraulic conductivity and hydraulic head as a function of soil moisture content in an unsaturated soil. However, for a more simplified approach, a volumetric/mass balance analysis (principle of continuity) may be used and which can be applied on a layered basis depending on soil and hydrogeological conditions. This latter approach conceptualizes each hydrogeological layer as a volume into which nutrient and water may be input until a threshold is reached and discharge (into the next layer) occurs. The requirements for detailed soil, nutrientand hydrogeological data render these models more difficult to apply and sensitive to the values of the parameters employed. Nevertheless, at the field scale, properly applied, they provide good simulation of the impacts on a given groundwater body. The three models considered here for nutrient transport based on processs simulation are: CREAMS/GLEAMS, see section 3.3.4, LEACHP/LEACHN, DAISY, SOIL/SOILN

In summary, the loading models are a fundamental part of the system treating the source as including deposition and the near-surface soil zone. This conceptualization in itself can be used as a screening tool for defining likely impacts on a groundwater body/aquifer, providing the relevant model is validated against field measurements initially. The process-based models are much more detailed in their approaches to contaminant migration, treating in detail the soil, hydrological and contaminant properties spatially and temporally. By their nature, they are data-hungry and often time-consuming in application. Parameter sensitivity is also reported as a common difficulty. Nevertheless, most are one-dimensional and only a few treat the dynamics of the receiving environment (saturated groundwater) specifically. Both loading and process-based models (e.g. NCYCLE, ANIMO and DAISY), may form part of larger suites of models for full catchment simulation models in which the receptor is usually surface water. Where groundwater body is the receptor, the level of detailed process simulation required in a model depends on the sensitivity of the receptor itself and the objectives of the investigation.

5.19.Identification and reversal of upward trends in groundwater pollutants

Environmental objectives for groundwater include measures to be implemented to reverse any significant and sustained anthropogenically induced upward trend in the concentration of any pollutant (Annex V, 2.4.4). In addition, surveillance monitoring is to provide information for use in the assessment of long term trends as a result of changes in natural conditions. The Commission itself is to publish criteria for the identification of trends and for the definition of starting points for trend reversal (Article 17).

A guidance report, Statistical aspects of the identification of groundwater pollution trends, and aggregation of monitoring results, has been published arising from a working group lead by the Austrian Federal Environment Agency (FEA), and initiated by the EU to develop guidance on specific issues of WFD implementation. The Irish EPA were represented in this working group. This project focuses on the development of statistical methods for the identification of trends and trend reversal in pollutants at the groundwater body level, including the determination of the minimum requirements for calculation, as well as a data aggregation method for interpretations and presentation of groundwater chemical status as defined in Annex V 2.4.5. The full report is available at http:\\www.wfdgw.net.

CHAPTER 6 MODELS AS DECISION SUPPORT TOOLS

6.1 Introduction

The first five chapters of this report describe: a general framework (DPSIR) to guide modelling (Chapter 1), the use of GIS as an essential element in the management of spatial data (Chapter 2) and the application of a wide range of models to a large and varied need (Chapters 3-5). This final chapter addresses the incorporation of models into catchment management as decision support tools. Appropriate use of models provides an important tool to support WFD implementation and meaningful dialogue among stakeholders.

The Water Framework Directive contains a number of technical requirements that necessitate scientific support. The specifications of these are outlined mainly in Article 5 (Characteristics of the River Basin District) and its associated Annex II, Article 8 (Monitoring of water status) and its associated Annex V, Article 11 (Programmes of Measures), Article 16 (strategies against pollution of water) that addresses listed substances, and Article 17 (strategies to prevent and control pollution of groundwater) and its associated, and forthcoming Groundwater daughter directive. Modelling is a likely feature of implementation of all of these Articles and can support the overall objectives of the WFD (Article 1) to meet the environmental objectives outlined in Article 4. Owing to time and cost constraints, modelling effort should be focussed to meet well-defined requirements. Where there is broad consensus on the measures that are needed to retain or improve ecological quality, models can help confirm the likely effectiveness of measures. Where there is no such consensus, modelling may be used as a tool to explore options and to faciliate discussions aimed at reaching consensus. This does not negate the additional use and development of models to address research goals in order to further understanding of catchment processes, but this should be seen as outside the immediate remit of WFD implementation. The prime objective of the WFD is not the understanding *per se* of the complexities of e.g. hydrological pathways, ecological response to pollution and alterations to hydromorphology but the protection or restoration of aquatic systems and terrestrial habitats that depend on them. Science has a role where current understanding limits management objectives, and in those circumstances modelling may be a valuable, and perhaps essential, support mechanism. Use of models must be appropriate to particular issues and scales, cost effective and sufficiently embedded in the River Basin Management systems to comprise an integral part of the River Basin Management Plans. This includes essential preliminary activities such as characterisation of the catchment, the risk assessment process and design of monitoring programmes, that lead to those plans. Where modelling does have a role it is, furthermore, not an end in itself but only part of the decision making process.

6.2 Science, policy and modelling

The WFD provides for an integrated approach to catchment management that, while widely accepted, is bedevilled by scientific, socio-economic and administrative complexities. Integration requires a broad appreciation, though not necessarily wholehearted acceptance, of a range of views. Environmental policy attempts to reflect current accepted understanding of pressures and impacts. For some sectors these provisions are well developed and exemplified by legal provision for Integrated Pollution Control Licences (Directive 96/61/EEC) and Environmental Impact Assessment (Directives 85/337/EEC, 97/11/EC). For other sectors there is unregulated provision for *good practice* or promotion of Environmental Management Systems (e.g. EEC Regulation 1836/93). The WFD goes beyond this, through general requirements to *inter alia* identify risks to surface and groundwater status, to prevent deterioration of waters and to restore status of water that fail to meet the Environmental Objectives.

The WFD provide normative but not definite definitions of many terms and there is a need for technical expertise to provide quantified and testable numbers to these. This process in itself will provide a requirement for the establishment of regional institutions (the RBDs) that will lead to furtherance in the understanding of catchment processes and management (Kallis and Butler, 2001). Clarification and development of the technical needs of the WFD have been the subject of much discussion leading to the publication of guidance documents to aid a Common Implementation Strategy across the Member States (see e.g. http://www.wfdireland.ie/ for further information and http://forum.europa.eu.int/Public/irc/env/wfd/library for direct access to Guidance documents).

For many of the technical requirements, there is an obvious need to support policies with a quantified approach, reminiscent of the words of William Thompson Kelvin:

“When you can measure what you are talking about, and express it in numbers, you know something about it; when you cannot express it in numbers your knowledge is of a meagre and unsatisfactory kind”

Quantification of natural states and processes include uncertainty, which can be accentuated in models that link processes together and incorporate insufficiently validated assumptions. The robustness of application of models to catchment management requires, at least, an awareness of model uncertainty. This can be particularly problematic for simulation models of ecosystems (Haag & Kaupenjohann, 2000). Uncertainty *per se* should not prevent the use of models; although if estimates of uncertainty are not included in measurement of inputs or dissemination of results it can undermine confidence in the process. Uncertainty should temper the interpretation and use of model outputs. There is, however, a seemingly common failure in the capacity of policy-makers and end-users to appreciate the uncertain nature of the natural world. This can lead to unrealistic demands for certainty and distraction among stakeholders about definitions of the problem to be solved (Webber, 1973).

Recent progress and foreseeable developments in dealing with uncertainty and increasing general acceptance of uncertainty in the natural world through decision support mechanisms will facilitate the incorporation of modelling techniques in catchment management. These developments will include increased use of probability analyses, such as Monte Carlo simulations and use of Baysian techniques that incorporates probabilistic reasoning and other imprecise methods such as fuzzy logic in models (Reichert, 1997). Use of such techniques requires increased technical know-how and training in their application to real situations. When operators and decision makers remain uncomfortable with complicated tools, the application of the most appropriate techniques may not occur.

Integration of science within policy and its effectiveness in day-to-day management requires enhanced methods of communication and understanding among scientists, decision makers and stakeholders. This approach is encapsulated by Lee (1993): "Managing large ecosystems should not rely merely on Science but on Civic Science; it should be irreducibly public in the way responsibilities are exercised, intrinsically technical, and open to learning from errors and profiting from successes".

The WFD promotes Civic Science. It requires an open approach to information exchange among all parties and a new vision to effect meaningful integration. Technical and financial limits accentuate the challenge. This process of *Integrated Environmental Assessment* promoted by the European Environment Agency (NERI, 1997) has been defined as:

"The interdisciplinary process of identification, analysis and appraisal of all relevant natural and human processes and their interactions which determine both the current and future state of environmental quality, and resources, on appropriate spatial and temporal scales, thus facilitating the framing and implementation of policies and strategies".

The use of mathematical models within this framework also requires a transcendence of scales and disciplines. Traditionally, scientists develop and run models within well defined domains of applicability (as discussed in Chapter 3), and the need for integration of scales and, particularly, disciplines can restrict model use. Models that have been developed at the plot or field scale cannot be automatically applied at the catchment scale without serious consideration of suitability, robustness and reliability. There is increasing recognition that heterogeneous catchments require a range of modelling approaches, with data collections made at appropriate spatial and temporal scales (Langan *et al*., 1997; Neal, 1997; Heathwaite *et al*.; 2002; Wade *et al*.; 2001).

The resolution of some of the difficulties that arise from modelling and management at the cacthment scale, and strong multiple stakeholder interest requires concise presentation of the underlying conceptual model, supported by clearly interpreted data. Without this, application of models may not gain stakeholder acceptance, and investment of resources in complex models may be wasted. The greater involvement of Competent Authorities and catchment users in defining the need for a modelling approach to WFD implementation, the greater the probability that models can play a meaningful role in the process. In this context it is important that effective strategies for communication exist within River Basin Management Committees and for the wider interested public. This should include realistic expectation by all parties of what models can and cannot achieve. Two extremes are best avoided because they are generally untrue: either that models are inherently useless or that the model is a full and accurate representation of reality.

Difficulties in the science to policy interface can be eased if there are recognised protocols for when modelling may be applicable and transparency of the decision making process. Procedural standards can help this process by specifying the parties to be involved and setting out the overall rationale for use of models (Hagenah, 1999). Hofmann and Mitchell (1998) promote a model coined RESPECT in order to address difficulties in the decision making process and to mitigate conflict between decision makers and end-users. For instances where modelling has been used to guide management such a strategy can be highly cost-effective, and may be particularly important where models which are not explicit in their mechanics are employed.

6.3 Use of models in decision support

Catchment management requires the integration of scientific, environmental and socio-economic information. Often the information comes from different disciplines, is difficult to interpret, and usually incomplete (Malafant & Fordham, 1998). Many decisions made under the WFD will require:

- Support tools such as GIS and databases;
- Models; and
- Decision Support systems

For decision support, modelling can be very useful as an investigative tool to forecast the outcome of various scenarios and to develop integrated frameworks for management. Such frameworks integrate the most appropriate existing models, data and knowledge and are commonly employed at the regional scale. This is in keeping with the River Basin District approach of the WFD. Decision scenarios allows the exploration of the *probability* of impacts from alterations of current management and assists with policy development (Fordham & Malafant, 1995). They can be a powerful aid to decision making and concensus building (Schauser, Lewandowski and Hupfer, 2003). An important aspect of frameworks is the bringing together of interdisciplinary skills through stakeholder workshops in order to optimise the use of knowledge, propose realistic outcomes, and provide for more effective decision-making (Watson & Wadsworth, 1996).

Models can be used to both predict probability of success of management innovations and to guide current management in order to meet future targets. This will be particularly relevant to *Programmes of Measures* of the WFD. There is, however, often a reluctance or genuine difficulty in applying complex process models to management questions. The aspiration that process models can by-pass the need for calibration, using *in-situ* measurements at new sites has not been satisfactorily achieved and such models may be rarely used for generic support to end-users in data sparse situations (Trudgill and Ball, 1995). Only in conjunction with routine data collection, investigative monitoring, or through project-linked research in the operation of River Basin Management Projects, are these models likely to be useful to resource managers. Simpler management orientated models using functional or empirical relations appear more feasible, if less accurate, options. The simpler models generally lack the mechanistic detail of the process models and may provide less insight to the required, and targeted, solutions of any particular problem. However, even simple approaches, such as nutrient soil indexing (Gburek *et al*., 2000) may be time consuming and difficult to apply at catchment scales. In addition, management options are often quite crude and fail to address important differences in geochemistry within regions or even catchments. The choice to use simpler models over complex ones requires careful consideration, and there is no point in applying a simple model if it is inadequate for the task at hand. Many complex models that address water quality and quantity have undergone considerable development over the last twenty years to provide "user friendly front ends" and, where appropriate, such models should be employed.

Management often needs to utilise existing knowledge, through e.g. routine monitoring that occurs at scales and includes variables not wholly appropriate to the salient catchment processes. The use of "meta-models" permits simplified input from complex mechanistic models (Brooks *et al*., 2001; Jarvis *et al*., 1997) that may provide a generic and generally more useable modelling framework. Examples applicable to estimation of nutrient loss to water are SOILNBD (Johnsson *et al*., 2002), MAGPIE (Lord and Anthony, 2000), TOPMODEL and P-Tools (Heathwaite, 2003; Heathwaite *et al*., 2003a). Further development of modelling frameworks will link distinct models at the catchment scale. Examples include the STONE model (Wolf *et al*., 2003) that consists of a chain of models integrated in order to evaluate effects of changes in agriculture in response to policy needs on emission of nutrients to surface and groundwaters, efforts to link SOILNBD link with the hydrological model HBV-N (Johnsson *et al*., 2002) and the module nature of the SOBEX models (www.sobek.nl). At a more generic level, scenario modelling packages such as *What if* (Veitch *et al*., 1993) incorporate both scientifically derived models and sociological aspects within a structured debate using expert judgement to develop integrated modelling frameworks (Luiten, 1999). These help identify common goals among research providers and users (Heathwaith, 2003). Current work under the EU HARMONIT project addresses linking of mathematical computer codes in order to develop a common open modelling interface (Reed *et al*., 1999) applicable to the WFD. Focus is currently on hydrological models (Gijsbers, 2003).

A key point in the application of mathematical models to support the implementation of the WFD is that they should be useful and relevant to management objectives, which themselves need to be well defined. While the implementation of the WFD requires input and action from a variety of sources, the information provided by science, often through model use, needs to be sufficiently reliable. Poor use of science or models undermines the implementation process. Models can assist conflict resolution. Implementation of River Basin Management Plans that includes model use also requires a system of user support in order to avoid inappropriate model use and interpretation. Well defined use of models, well developed software and good in-house or on-line support reduces the need for users' technical skills. Lack of numerate young scientists in Ireland is, however, recognised as a limitation to national development of modelling skills (Elliott, 2001). The realities of limitations on budget and available expertise, at least during the early stages of implementation of the WFD may restrict application of the more complicated models, even if these are appropriate tools in the circumstances. Choice of models can be aided by decision trees (chapter 3, Figure 3. 10 and 3.11) for optimal model use (Somlyody, 1997).

Generic simulation tools such as STELLA are also helpful for identifying the connections among catchment components and processes and, hence, modelling needs. Recent development of the ECOPATH model (Christensen et al., 2000) allows simulations of different management scenarios and their likely impact on the structure and productivity of the system (ECOSIM scenarios). Ecosim has been proposed as a tool that can be used for "study of [fishery] response dynamics in any ecosystem for which there are sufficient data to construct a simple mass-balance model" (Walters, 1997). While these tools are being increasingly used for estimation of trophic dynamics in inshore fisheries they are not commonly used in catchment management. Their potential could be high in application of modelling to the WFD.

Mechanistic simulation models of ecosystems as reliable tools may, however, be limited because while the mathematical conceptualisation is computable, it is of necessity a simplification of the natural system and may not include some important behaviour modes. In particular, the self-modifying character of ecosystems is not easily represented by a dynamical system. While the view of Haag & Kaupenjohann (2000) that to embrace the complexity of natural systems requires abandoning prediction modelling and adopting more fully a precautionary principle rather that an expectation of ecosystem engineering may not be a universal one, it does illustrate inherent difficulties in application of ecological models to management. This difficulty arises, in general, because ecological models have been developed and used primarily for research, rather than management, objectives. Increased understanding of complex systems without robust and generally applicable results may satisfy the researcher, but not the manager. The gulf between research and application has also resulted often in poor model documentation and prompted a standardised and accessible documentation of ecological models (Benz and Knorrenschild, 1997; Hoch *et al*., 1998) found at the Register of Ecological Models (http://www.wiz.uni-kassel.de/ecobas.html). Quality Assurance protocols are also generally less well developed for ecological than for many hydrological and groundwater models (Refsgaard, 2002).

6.4 Key components of the Directive where modelling is likely of use.

The potential use of mathematical models in the implementation of the WFD is clearly large. It is not possible from this review or from the information currently being collected in large EU funded programmes (e.g. BMW, http://www.vyh.fi/eng/research/euproj/bmw/homepage.htm) to identify individual models as the most superior in any particular context. Indeed, comparison of models applied to the same situation is uncommon (e.g. Valiela *et al.*, 2002; Letcher *et al.*, 2002; also see EUROHARP, http://www.euroharp.org/index.htm). However, current ERTDI EPA projects, such as 2000LS 2.2 are addressing this need in the area of phosphorus modelling, but the final results from such projects will become available only after the publication of this report. Large variability of outputs across models is not uncommon. More complex models may be more responsive and precise, but not necessarily more accurate or predictive (Valiela *et al.*, 2002). Recommendations for appropriate model use relate, therefore, to principles rather than specifics. Modelling is likely to be highly applicable and cost effective for a number of the early milestones of the WFD (Table 6.1.). As the process of WFD implementation in refined in the future, so too will be the contribution of modelling

Table 6.1. Likely areas where application of mathematical models can assist with fulfilment of early tasks identified as necessary towards implementation of the WFD, with dates for progress milestone (P.Duggan, DOEHLG, pers com.) and external delivery. Delivery dates are December, unless otherwise stated

Task	Milestone	Delivery/operational date	Relevant WFD Article
GIS mapping of catchments and water bodies	2004 (June)	2004	5
Intercallibration exercise	2003	2006 (June)	5
Determine typology and reference conditions	2004 (June)	2004	5
Risk assessment	2004 (June)	2004	5
Ecological classification	2005 (Sept)	2006	8
Design monitoring systems and network	2004 (June)	2006	8
Consult stakeholders	2006	2008	14
Identify programmes of measures	2005 (Mar)	2009	11

Chapter 3 provides a number of recommendations with regard to use and development of models. The need to prioritise modelling needs is obvious, but opinion on that among all interested parties will almost certainly vary, and require discussion. It is the view of the authors of this report that current modelling techniques are likely to be of particular importance for the implementation of the WFD in respect of:

- Identification of risk to ecological quality from catchment pressures. This should form part of the Characterisation process and relates to the legal requirement to identify water bodies that are at risk of failing to reach environmental objectives. It will use recent developments in GIS coverage*;*
- Hydrological regimes and estimation of annual nutrient loads;
- Assistance with elucidation, assessment and choice of *Programmes of Measures*, which necessitates a case-by-case approach; and
- Definition of spatial and temporal resolution of monitoring systems for identification of hydromorphology, and chemical and ecological status;

Further developments of modelling are required to assist with:

- Determination of reference conditions and methodology for determining departure from reference state and Ecological Quality Ratios (EQR);
- Use of artificial intelligence techniques for assisting with determination of EQRs;
- Identification of appropriate temporal and spatial scales to model impact of catchment processes on pollutant loads;
- Modelling frameworks for selection and integration of models;
- Development of decision and user support, to include enhanced communication for widespread understanding and use of models and dialogue among stakeholders; and
- Modelling of ecological systems response to s*tate* changes and management measures.

Focus on the requirements within the WFD, and current developments arising from the Common Implementation Strategy Groups, relevant to Risk Assessment and Monitoring and Classification merit further discussion.

6.5 A view of risk

Risk can be defined as the product of the probability of an event occurring and the consequences of that event. The assessment of risk is an important part of the characterisation process of catchments and in making judgements of the likelihood that water bodies will fail to meet defined environmental objectives. There is a key role for modelling risk in order to relate pressures to impacts. The CIS IMPRESS guidance document provides a detailed discussion of issues relevant to risk assessment and identification of pressures and impacts**.** Recent work by the Irish WFD National Implementation Strategy Group has summarised this. The partitioning of pathway susceptibility to pollutant mobility and receptor sensitivity to impact is important in the assessment of risk that water bodies will fail environmental objectives (Figure 6.1.).

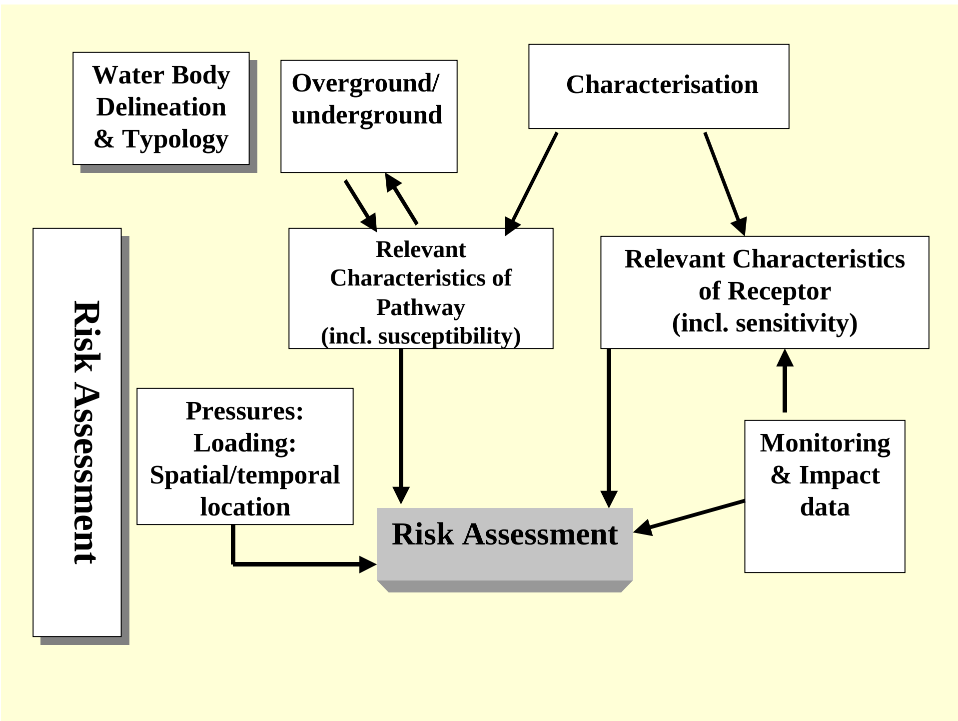

Figure 6.1. Schematic of relationship between River Basin characterisation and Risk assessment (Adapted from Daly, Kilroy & Glasgow/Willows and Carey)

Adoption of well-structured tools for assessment of risk, coupled with appropriate models, that can be applied easily to explore management scenarios and coupled to GIS, is recommended. Characterisation of catchments, initially required by the end of 2004, should incorporate simple models of risk assessment.

Risk can be modelled based on:

- Topographical, climate and soil characteristics-the simple map variables of Hakanson and Peters (1995);
- Activity risk; and
- Spatial pattern and proximity to risk (see (Soranno *et al.*, 1996; Heathwaite *et al.*, 2003)

This identifies key contributor and problem areas (Haag & Kaupenjohann, 2001). An example of a risk assessment methodology is the US P-index, a simple screening tool to help end-users identify agricultural areas or practices vulnerable to P loss (Sharpley *et al*., 1998). Ranking of source and transport factors, based on hydrology, soil P and management identifies risk of movement of P. The tool has, however, attracted criticism as quite crude and limited by e.g. precision of spatial and temporal information (Heathwaithe, 2003). Current research is focussed on evaluating incorporation of existing soil survey, topographic maps, stream channel networks and other GIS databases. The development of the use of such “static variables” is clearly important for estimation of risk of impact from pressures in the catchment (Hakanson, 1996; Heathwaith *et al*., 2003). Risk assessment and simple computation of nutrient budgets should guide monitoring. Seasonal models (see Jennings *et al*., 2003) can help the spatial resolution of that.

A conclusion of the IMPRESS CIS group was that the requirements of the WFD in relation to Pressures and Impacts are not simply met by the purchase and running of a “off the shelf” computer model, but that existing tools are probably sufficient to provide a reasonable assessment of risk that water bodies may fail the environmental objectives. This conclusion supports that of our review.

6.6 A view on monitoring

Surveillance monitoring under the WFD requires a monitoring network that is sufficiently sensitive to provide an overall assessment of water bodies and long-term changes. The WFD stipulates that surveillance monitoring is required for at least one year for parameters indicative of all biological, physicochemical and hydromorphological quality elements within each River Basin Plan. Assessment of water bodies that are deemed not to be at risk of failing to meet the environmental objectives and which have already been monitored in a preceding River Basin Plan need only be monitored as infrequently as once every 18 years. The first River Basin Plan would, therefore, appear to require the greatest extent of surveillance monitoring. The WFD does not, however, provide very useful advise on sampling frequencies. The guidance given in Annex V appears statistically naïve (CIS Monitoring WG, 2002). Monitoring needs to be within stated limits of confidence (the probability that the true value of a statistical parameter lies within the limits placed around an estimated mean from measurements) and precision (the divergence of the true and estimated parameter). In addition, the elements to be monitored are those *indicative* of quality. Monitoring the entire spectrum of e.g. biotic elements without regard to the reliability of the results is a waste of time and money. This has critical bearing for the validation of modelling outputs. Given the uncertainty in interpreting results owing to natural variation or difficulty of sampling methodologies, sampling programmes need clear objectives, thoughtful consideration of the variables measured and clear rationale for monitoring frequencies. None of these are easy demands. Design of surveillance monitoring systems and protocols can be assisted by modelling. This would include the use of GIS in order to identify the spatial network and ensure adequate representation of all typologies, the estimation of frequency distributions of collected data and the targeting of sampling through risk analysis sensitive to seasonal variation.

The principles outlined above apply equally to *operational monitoring,* which is required if there is a risk of failure to meet the environmental objectives. Monitoring guides the *Programmes of Measures.* The CIS Guidance on monitoring emphasises the importance that such monitoring provides:

- An assessment of the deviation from reference state;
- Provides for natural and artificial physical habitat variation;
- Accounts for the range of natural variability and variability arising from anthropogenic activities of all quality elements in all water body types;
- Accounts for the interactions between surface and groundwaters; and
- Provides for the detection of the full range of potential impacts to enable a robust classification of ecological status.

Operational monitoring needs to be targeted in order to be cost-effective. It is the view of the CIS group that operational monitoring can be targeted to water bodies that are representative of particular pressures and typologies to be monitored, rather than all bodies at risk. In general for all monitoring a greater frequency is required for *Protected Areas.* The WFD also refers to the need for *Investigative monitoring.* This is required to determine where reasons for failure to meet objectives are uncertain and to assess impact of accidental pollution. Some of the more complex and process models are likely to be needed in these circumstances in order to identify e.g. pollutant pathways and remediation strategies.

Monitoring frequency should be determined by natural variability and risk of misclassification. Errors around modelling and monitoring outputs can lead to a misclassification of a waterbody's status. Discussion of this issue is provided in the CIS documents on Monitoring and Reference conditions (REFCOND) and, further, by the second generation CIS Working Group ECOSTAT, which draws upon the results of the previous deliberations. This is a crucial area with respect the implementation of the WFD which requires further research and development. The statistical considerations for reporting results, risks of misclassification of a site and decisions on how many elements will be included in an individual assessment of a single or group of water bodies are issues that require both case-by-case decisions <u>and</u> general agreement on the principles that will be adopted within and among River Basin Districts. These discussions should be based on statistical treatment of data in order to guide monitoring objectives. Strategies would usefully be integrated into that process and not be considered as an activity set apart from monitoring.

Monitoring results lead to determination of Ecological Quality Ratios (EQR) for individual or clusters of sites. The current view of the ECOSTAT Working Group is that site classification will be based on the lowest EQR of all elements used in the determination. The greater the number of quality elements used to determine an overall EQR, then the greater will be the probability that reporting will downgrade the status of a site. The outcome can also be dominated by the quality element with the largest errors. The implication for reporting and, hence, the view of water body classification is obvious. It will be desirable for statistical reasons to reduce the number of elements considered. A reduction of elements produces, paradoxically a less holistic approach. Reliable reporting is, therefore, a major challenge for the implementation of the WFD and the application and interpretation of models that summarise large data sets in order to derive departure from reference condition need to pay particular attention to issues of robustness and reliability.

Models can, however, help with the development of determination of EQRs in the first place. Indeed, it could be argued that the most critical need for modelling for implementation of the WFD is directed towards the estimation of reference conditions. All other considerations of the assessment of waterbody quality stem from that. Response of ecological communities to impacts are not linear, so neither should the setting and increments of quality class boundaries. Determination of response-dose relationships in waterbodies is, therefore, required. It might be in that realm that development of ecological models will be also of particular importance.

A management response is required if the ecological status of a water body is determined to be less than good or, through monitoring, to have reduced between monitoring periods. A response necessitates a *Programme of Measures.* This requires the identification of the mechanism or mechanisms within the sequence of Pressures-State-Impact where remedial action is required. Mathematical models can guide the formation of *Programmes of Measures*. By the same token if overall EQR is acceptable, there would appear little motivation for detailed investigation using modelling or not unless there is reasonable probability of future deterioration of a waterbody owing to e.g. lag-times between pressure and impact. Such a possibility should, nevertheless, be encapsulated in risk analysis. Modelling for the WFD can, therefore, be particularly useful for a) risk assessment and b) investigative monitoring.

6.7 Overall Conclusions

In Europe, the US and Australia there is considerable activity in developing models and adapting models to catchment management. The WFD has set Environmental Objectives relevant for all catchments, and hence all activities, in Europe. The challenges of the WFD are significant and judicious use of mathematical models can help meet them. Like the integrated nature of the catchment or the WFD documentation, models provide one component of a much larger whole. Ultimately, it will be good management of catchment activities that reduces the risk of pollutant emission that will play the most significant role in the protection of European water resources. These principles are employed in industrial Environmental Management Systems, and translation to the context of catchment management makes complete sense. However, while there is uncertainty about the nature of pollutant movement through catchments, their impact on receiving water bodies and the consequence on ecological communities of hydromorphological and chemical alterations, modelling can assist management.

This report has identified many areas where modelling can be usefully employed. Through a series of recommendations and final discussion it has highlighted where modelling can be effectively used, where further development is required and where it fits in within the overall implementation of the WFD. In summary and final conclusion the following are key issues:

- Models are, by nature, simplifications of reality;
- Management objectives need to be defined clearly to guide model use;
- There are no universal models, and selection of appropriate models for specific tasks is critical;
- Models are likely to be extremely valuable in the assessment of risk of water bodies failing to meet environmental objectives and in *investigative monitoring.*
- Risk assessment should employ models to target monitoring and *Programmes of Measures;*

- Simple models are, generally, more likely to be used and understood than complex ones, but great care is needed to avoid inappropriate model use. Complex models applied with the necessary expertise or user support can be far superior where there is a need to address spatial and temporal complexities;
- There needs to be an appreciation of the strengths, weaknesses and uncertainties of individual models, where used;
- All models, and the measurements used to calibrate and validate them, have errors which need to be quantified and reported;
- Catchment and hydrological models are generally more well developed, and with greater consensus of applicability to the WFD, than ecological models;
- As determination, prevention and reduction of impact are the pillars of the WFD, there needs to be a greater emphasis on the development and application of ecological models to support the implementation of the WFD;
- The determination of reference conditions and EQRs across water body typologies provides a major challenge for which the development and application of models can be usefully targeted.

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Appendix I

Contents of Appendix I:

Abbreviation	Model title	Webpage
AGNPS	AGricultural Non Point Source Pollution Model	http://www.sedlab.olemiss.edu/agnps.html
ANIMO	Agricultural Nutrient Model	http://www.alterra.nl/english/default.asp
ANNEX	Annual Network Nutrient EXport	
ANSWERS	Areal Nonpoint Source Watershed Environment Response Simulation	
AQEM	The Development and Testing of an Integrated Assessment System for the Ecological Quality of Streams and Rivers throughout Europe using Benthic Macroinvertebrates	http://www.aqem.de/
AQUATOX	A simulation model for aquatic ecosystems	http://www.epa.gov/waterscience/models/aquatox/
AUSRIVAS	Australian RIVer Assessment System	http://ausrivas.canberra.edu.au/
BASINS	Better Assessment Science INtegrating Point and Nonpoint Sources	http://www.epa.gov/waterscience/basins/basinsv3.htm
BATHTUB		http://www.wes.army.mil/el/elmodels/emiinfo.html
BEAST	Benthic Assessment of Sediment	http://www.ec.gc.ca/ceqg-rcqe/English/Html/SAS/factsheet_3.cfm
BMWP	Biological Monitoring Working Party System	http://lakes.chebucto.org/ZOOBENTH/biotic.html - BMWP
CATCHMOD	Catchment Modelling Cluster	http://www.harmonit.org/links/catchmod.htm
CATS-5	*C*ontaminant in *A*quatic and *T*errestrial eco*S*ystems	
CE-QUAL-W2	A hydrodynamic and water quality model for rivers, estuaries, lakes, and reservoirs	http://www.wes.army.mil/el/elmodels/w2info.html
CONDUIT FLOW		
CORINE	Co-ORdination of INformation on the Environment	http://www.eea.eu.int/
CORMIX	CORnell MIXing zone model	http://www.cormix.info/
CREAMS	Chemicals, Runoff, and Erosion from Agricultural Management Systems	http://dino.wiz.uni-kassel.de/model_db/mdb/creams.html
DAISY	Soil-plant system model	http://www.dina.kvl.dk/~daisy/
DATBAL		http://www.cbl.cees.edu/~ulan/ntwk/network.html

DARCY'S LAW		
DHRAM	Dundee Hydrological Regime Assessment Method	
DIVAST	Depth Integrated Velocity And Solute Transport	http://www.engin.cf.ac.uk/research/summary.asp?GroupNo=3
DRAINMOD	Methods for Design and Evaluation of Drainage-Water Management Systems for Soils with High Water Tables	http://www.bae.ncsu.edu/soil_water/drainmod/
DR3M-QUAL	Distributed Routing Rainfall Runoff Model—Quality	http://water.usgs.gov/cgi-bin/man_wrdapp?dr3m
ECOHAM	Ecological North Sea Model Hamburg	http://www.ifm.uni-hamburg.de/~wwwem/dow/Ecoham/
ECOMSED	Estuarine and Coastal Ocean Model + SEDiment Transport	http://www.hydroqual.com/Hydro/ecomsed/
ECOPATH		http://www.ecopath.org/
ECOSIM	ECOsystem SIMulation	http://www.isima.fr/ecosim/
EPIC	Erosion-Productivity Impact Calculator	http://www.brc.tamus.edu/epic/
ERSEM	European Regional Seas Ecosystem Model	http://www.nioz.nl/en/deps/bio/projects/ERSEM/Description.html
EUROHARP	European Harmonised Procedures for Quantification of Nutrient Losses from Diffuse Sources	http://www.euroharp.org/
EUTROMOD	Evaluation of the Water Quality Model	http://www.nalms.org/bkstore/software.htm
EVHA	Logiciel d'EValuation de l'Habitat	http://www.lyon.cemagref.fr/bea/lhq/software.html
FLOWPATH II		http://www.flowpath.com/software/software_main.htm
FLUX	Simplified Procedures for Eutrophication Assessment and Prediction	http://www.wes.army.mil/el/elmodels/emiinfo.html
GBMBS	*G*reen *B*ay *M*ass *B*alance *S*tudy	http://www.epa.gov/grtlakes/gbdata/
GLEAMS	Groundwater Loading Effects of Agricultural Management Systems	http://www.ars.usda.gov/research/publications/publications.htm?SEQ_NO_115=104920
GROUNDWATER VISTAS		http://www.groundwatermodels.com/software/Software.asp
GLUE	Generalised Likelihood Uncertainty Estimation	http://www.es.lancs.ac.uk/hfdg/glue.html
GWLF	Generalised Watershed Loading Function	

HBV-N		http://www.smhi.se/sgn0106/if/hydrologi/quality.htm
HARMONIQUA	Harmonising Quality Assurance in model based catchment and river basin management 2002-2005	http://harmoniqua.wau.nl/
HEC	Hydrologic Engineering Center	http://www.hec.usace.army.mil/default.html
HOC BIOACCUM-ULATION	Model for shallow aquatic systems	
HSCTM2D	Hydrodynamic, Sediment and Contaminant Transport Model	http://www.epa.gov/ceampubl/swater/hsctm2d/
HSPF	Hydrological Simulation Program—Fortran	http://water.usgs.gov/software/hspf.html
HYDROTEL		http://www.hydrotel2000.com/
IHACRES	Identification of unit hydrographs and component flows from rainfall, evaporation and streamflow data	http://dataserv.cetp.ipsl.fr/AIMWATER/hydromodels/IHACRES.html
INCA	Integrated Catchment Model	http://www.reading.ac.uk/INCA
LOICZ		http://www.nioz.nl/loicz/
MAGPIE	Modelling Agricultural Pollution and Interactions with the Environment	
MIKE 11	Hydrodynamic Model	http://www.dhisoftware.com/mike11/
MIKE 21	Hydrodynamic Model	http://www.dhisoftware.com/mike21/
MLF	Micro Low Flows	http://www.nwl.ac.uk/ih/www/products/iproducts.html
MODFLOW		http://water.usgs.gov/nrp/gwsoftware
MODPATH		http://water.usgs.gov/nrp/gwsoftware
MT3D99		http://www.scisoftware.com
N CYCLE	Nitrogen Cycle	http://www.clues.abdn.ac.uk:8080/mert_idx.html.
NLEAP	Nitrate Leaching and Economic Analysis Package	http://gpsr.ars.usda.gov/products/nleap/nleap.htm
N-LES	Nitrate Leaching EStimator	http://www.euroharp.org/pd/pd/models/Nles-short.htm
NTWRK	Analysis of Ecological Flow Networks	http://www.cbl.cees.edu/~ulan/ntwk/network.html
PAEQANN	Predicting Aquatic Ecosystem Quality using Artificial Neural Networks	http://www.fundp.ac.be/urbo/paeqann.html

PHABSIM	Physical HAbitat SIMulation	http://www.fort.usgs.gov/products/software/phabsim/phabsim.asp
PHOSMOD		http://www.nalms.org/bkstore/software.htm
PLUME-RW	Pollutant dispersion	http://www.hrwallingford.co.uk/software/telemac.html - top
PLUMES		http://www.epa.gov/ceampubl/swater/plumes/
POM	Princeton Ocean Model	http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/
PROFILE		http://www.wes.army.mil/el/elmodels/emiinfo.html
PROTECH	Phytoplankton RespOnses To Environmental Control	http://windermere.ceh.ac.uk/algalmodelling/contents/ProtechC/ProtechCPage.htm
QWASI	*Q*uantitative *W*ater, *A*ir and *S*ediment *I*nteraction	http://www.trentu.ca/cemc/models/Qwasi.html (first version)
RAM		http://www.groundwatermodels.com/software/SoftwareDesc.asp?software_desc_id=75&software_id=10
REGCEL	Water level analysis	
RHABSIM	Riverine HABitat SIMulation	http://www.northcoast.com/~trpa/
RHS	River Habitat Survey	
RIVPACS	River InVertebrate Prediction And Classification System	http://www.dorset.ceh.ac.uk/our_science/General Sections/waterquality/Rivpacs_2003/rivpacs_introduction.htm
RZWQM	Root Zone Water Quality Model	http://gpsr.ars.usda.gov/products/rzwqm.htm
SED3D	Three-Dimensional Numerical Model of Hydrodynamics and Sediment	http://www.epa.gov/ceampubl/swater/sed3d
SHE	Système Hydrologique Européen	
SMIC	Surface Water and Water Quality Models Information Clearinghouse	http://smig.usgs.gov/SMIC/SMIC.html
SOBEC		http://www.sobek.nl
SOIL	simulation model for soil water movement and heat	
SOIL-N	simulation model for nitrogen conditions in soils	http://amov.ce.kth.se/AMOVNew.htm#5
SPARROW		http://water.usgs.gov/nawqa/sparrow/intro/intro.html
STONE		http://www.alterra.nl/models/stone/p_stone_model.htm
SWAT	Soil and Water Assessment Tool	http://www.brc.tamus.edu/swat/

SWIM	Soil and Water Integrated Model	http://www.brc.tamus.edu/swat/othermod/swim-des5p.htm
SWMM	Storm Water Management Model	http://ccee.oregonstate.edu/swmm
SWRRB	Simulator for Water Resources in Rural Basins	http://abe.www.ecn.purdue.edu/~wepphtml/wepp/wepptut/jhtml/swrrb.html
TELEMAC	Numerical modelling system for free surface hydrodynamics, sedimentology, water quality, waves and underground flows	http://www.telemacsystem.com/
TOPMODEL		http://www.es.lancs.ac.uk/hfdg/topmodel.html
TRK	The Swedish System	http://www.euroharp.org/pd/pd/models/TRK-short.htm
VISUAL PLUMES	Dilution models for effluent discharges	http://www.epa.gov/ceampubl/swater/vplume/index.htm
WASP	Water quality Analysis Simulation Program	http://www.epa.gov/ceampubl/swater/wasp/index.htm

AGNPS — AGricultural Non-Point Source Pollution Model

Description:
AGNPS is a joint USDA-Agricultural Research Service and Natural Resources Conservation Service system of computer models developed to predict non point source pollutant loadings within agricultural watersheds. It contains a continuous simulation, surface runoff model designed to assist with determining BMPs, the setting of TMDLs, and for risk & cost/benefit analyses.

Data Requirement:
The input programs include: (1) a GIS-assisted computer program (TOPAZ with an interface to AGNPS) to develop terrain-following cells with all the needed hydrologic & hydraulic parameters that can be calculated from readily available DEM's; (2) an input editor to initialise, complete, and/or revise the input data; and (3) an AGNPS-to-AnnAGNPS converter for the input data sets of the old single-event versions of AGNPS (4.03 & 5.00). AnnAGNPS includes up-to-date technology as well as the daily features necessary for continuous simulation in a watershed.

Output:
The model provides estimates of: (1) hydrology, with estimates of both runoff volume and peak runoff rate; (2) sediment, with estimates of upland erosion, channel erosion, and sediment yield; and nutrients (both sediment attached and dissolved), with estimates of pollution loadings to receiving cells. A graphics option in the program allows the user to plot different variables within the watershed.

Version and System Requirements:
The program is written in standard FORTRAN 77 and has been installed on IBM PC/AT and compatibles. A hard disk is required for operation of the programme and a math co-processor is highly recommended. Executable code prepared with Ryan-McFarland compiler and is available only for MS/DOS environment. Source code is only available for MS/DOS environment.

Assumptions and Limitations:
The model does not handle pesticides. The pollutant transport component needs further field testing. Nutrient transformation and instream processes are not within model capabilities.

Application History:
The model is being used extensively within United States to evaluate non-point source pollution by various government agencies and consultants. Setia and Magleby (1987) used AGNPS for evaluating the economic effect of non-point pollution control alternatives. The model has also been used by Koelliker and Humbert (1989) for water quality planning. APNPS was used by Frevert and Crowder (1987) to analyse agricultural non-point pollution control options in the St. Albans Bay watershed.

Availability:
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Website:
http://www.sedlab.olemiss.edu/agnps.html

ANIMO — Agricultural Nutrient MOdel

Description:
ANIMO dynamically simulates the carbon, nitrogen and phosphorus cycles in unsaturated and saturated soil systems. The model was developed to analyse the leaching of nitrogen from the soil surface to groundwater and surface water. Optional simulation of the phosphorus cycle has been added to the model.

Data Requirement:
An extended soil water balance, fertilizer management (amount, kind of fertilizer, time and depth pf application), soil physical properties (pF, bulk density, five temperature parameters, diffusion coefficient for oxygen in soil), soil chemical properties (pH, sorption coefficients, sorption rates), boundary and initial conditions.

Output:
All terms of complete balances of a soil-water-crop system for water, nitrate-N, ammonium-N, organic-N, ortho-N, organic-P.

Version and System Requirements:
VAX, IBM-compatibles with coprocessor. Programming language: FORTRAN

Assumptions and Limitations:
The model system is a multi-layer one-dimensional soil column. The upper boundary is the soil surface, the lower boundary is the depth of the local groundwater flow and the lateral boundary is defined by the surface water system(s). Main processes included in the model are: mineralisation and immobilisation, crop uptake, denitrification related to (partial and temporal) anaerobiosis and decomposing organic materials, oxygen and temperature distribution in the soil, nitrification, desorption and adsorption of ammonium and phosphorus to the soil complex, runoff, discharge to different surface water systems and leaching groundwater.

ANIMO was developed for the Dutch situation and an erosion component was not included. The model does not contain a hydrological model, but needs external hydrological information to calculate the transport processes. The model has been linked with the DEMGEN model.

Application History:
The majority of model applications have been limited to Dutch sites. The model has also been applied for regional assessments.

Availability:
Main contact:

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Website:

http://www.alterra.nl/english/default.asp

ANNEX **Annual Network Nutrient EXport**

Description:
The model sums nutrient sources delivered to each link of a river network, and accumulates the consequent loads to determine average annual exports:
- Combines soil nutrient concentrations from Australian Soil Resources Information System with estimates of average annual sediment loads from SedNet modelling to estimate the average annual nutrient loads to rivers associated with water erosion.
- Combines estimates of average annual nutrient loads for surface run-off from BIOS modelling with point source data from the National Pollutant Inventory (http://www.environment.gov.au/epg/npi/database/database.html) to estimate the average annual loads of dissolved nutrient to rivers. ANNEX also models the exchange of phosphorus between the suspended sediment and dissolved forms. This process is described by an adsorption coefficient (Ks) that expresses changes in particulate phosphorus concentrations as a ratio of the resulting proportional change in dissolved phosphorus concentrations. *Ks* is largely determined by sediment particle size and mineralogy. The model assumes that: The concentration of phosphorus adsorbed to the suspended sediment is in equilibrium with the dissolved phosphorus concentration; the system is in steady-state; phosphorus transport associated with phytoplankton is a small component of the total budget; and there is no exchange between dissolved and sediment-bound nitrogen. Loss of dissolved nitrogen by denitrification is modelled as an exponential decay process dependent on the residence time of flow in the network link, water temperature, and a rate constant that varies according to river substrate type

Assumptions and Limitations:
The model assumes that the: sediment-attached nutrient load is associated with the clay fraction of the sediment being transported entirely in suspension; and capacity for transport of nutrients both in dissolved forms and associated with suspended sediments is unlimited.

ANSWERS **Areal Nonpoint Source Watershed Environment Response Simulation**

Description:

ANSWERS was developed at the Agricultural Engineering Department of Purdue University (Beasley and Huggins, 1981). It is an event based, distributed parameter model capable of predicting the hydrologic and erosion response of agricultural watersheds. Application of ANSWERS requires that the watershed to be subdivided into a grid of square elements. Each element must be small enough so that all important parameter values within its boundaries are uniform. For a practical application element sizes range from one to four hectares. Within each element the model simulates the processes of interception, infiltration, surface storage, surface flow, subsurface drainage, and sediment drainage, and sediment detachment, transport, and deposition. The output from one element then becomes a source of input to an adjacent element. As the model is based on a modular programme structure it allows easier modification of existing programme code and/or addition of user supplied algorithms. Model parameter values are allowed to vary between elements, thus, any degree of spatial variability within the watershed is easily represented. Nutrients (nitrogen and phosphorus) are simulated using correlation relationships between chemical concentrations, sediment yield and runoff volume. A research version of the model uses "clay enrichment" information and a very descriptive phosphorus fate model to predict total, particulate, and soluble phosphorus yields.

Data Requirement:

Data need comprise detailed description of the watershed topography, drainage network, soils, and land use. Most of the data can be obtained from USDA-SCS soil surveys, land use and cropping surveys.

Output:
The model can evaluate alternative erosion control management practices for both agricultural land and construction sites (Dillaha *et al*., 1982). Output can be obtained on an element basis or for the entire watershed in terms of flow and sediment. The ANSWERS program comes with a plotting program.

Version and System Requirements:
The program is written in standard FORTRAN 77 and has been installed on IBM PC/AT and compatibles. A hard disk is required for operation of the programme and a math co-processor is highly recommended. Executable code prepared with Ryan-McFarland compiler.

Assumptions and Limitations:
The model does not deal with snow melt. It uses correlation equations between P and N and sediment loss to predict the losses of these chemicals. It does not model the transformation of either P and N as it moves through the catchment. It simulates single events only.

Application History:
The model has been successfully applied in Indiana on an agricultural watershed and a construction site to evaluate best management practices by Beasley (1986).

Availability:
To obtain copies of the model please write or call Dr. David Beasley at the following address:

Dr. David Beasley, Professor and Head

Dept. of Agricultural Engineering

University of Georgia

Coastal Plain Experiment Station

P.O. Box 748

Tifton, GA 31793

(912) 386-3377

or download at:

http://dillaha.bse.vt.edu/answers/index.htm

AQEM	The Development and Testing of an Integrated Assessment System for the Ecological Quality of Streams and Rivers throughout Europe using Benthic Macroinvertebrates

Description:
The AQEM assessment system is the main result of the European Union funded project AQEM, which was carried out from March 2000 to February 2002. It serves the implementation of the EU Water Framework Directive and provides a system for assessing ecological quality in European streams with benthic macroinvertebrates. Aims of the AQEM system are: 1) to classify a stream stretch in a quality class from 5 (high) to 1 (bad) based on a macroinvertebrate taxa list and 2) to give information about the cause of a possible degradation to help direct future management practices. In contrast to many other comparable projects, the development of the AQEM system has been based on a new dataset covering both the fauna and general stream characteristics of 28 common European stream types.

Version and System Requirements:
AQEM assessment software Version 2.1 is designed to assess the Ecological Quality of 28 European stream types based on macroinvertebrate taxa lists ('4th deliverable' of AQEM). AQEM dip software is a tool for storing both, macroinvertebrate taxa lists and data on stream characteristics, based on the Austrian software ECOPROF. The software is capable of storing all data recorded in the AQEM site protocol. It offers a large variety of export functions.

Availability and Website:
The AQEM assessment software Version 2.1, AQEM assessment software manual, AQEM manual and AQEM taxa list are available at:
http://www.aqem.de/

AQUATOX — A simulation model for aquatic ecosystems

Description:

AQUATOX is a freshwater ecosystem simulation model which predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants. The model simulates multiple environmental stressors (including nutrients, organic loadings and chemicals, and temperature) and their effects on the algal, macrophyte, invertebrate, and fish communities. Therefore, AQUATOX can help identify and understand the cause and effect relationships between chemical water quality, the physical environment, and aquatic life. The model can represent a variety of aquatic ecosystems, including: vertically stratified lakes; reservoirs and ponds and rivers and streams (Park *et al*., 1995).

Data Requirement:

AQUATOX comes bundled with data libraries that provide default data. This is of particular importance for the biological data, which are probably the most difficult for a user to obtain.

Required input data are:

- loadings[1] to the waterbody.
- general site characteristics.
- chemical characteristics of any organic toxicant.
- biological characteristics of the plants and animals.

[1] Environmental loadings can be from multiple sources such as: constant or dynamic; point or nonpoint sources; upstream contributions and atmospheric deposition.

Output:

AQUATOX provides output in terms of time varying biomass of the various plants and animal, chemical concentrations in water, and concentrations of the organic toxicant in water, organic sediments and biota. It has numerous features to assist in display and analysis of results: Graphing capability; Easy export to spreadsheet programs; Option to save time varying rates, such as consumption and photosynthesis and uncertainty and sensitivity analysis capability

Version and System Requirements:
Minimum: Pentium PC, 133 MHz; Windows 95, 98, 2000 or NT; 64 MB RAM and 30 MB free disk space.

Recommended: Pentium PC, 600MHz or higher; Windows NT, 2000 or XP; 128 MB RAM and 75 MB free disk space. In comparison to the previous versions of Aquatox distributed by the USEPA in release phase 1 and 1.1. The updated version has following enhancements:

- improved stream simulation, by allowing habitat differentiation, simulation of inorganic sediments, and loss of plant and animal biomass due to stream flow effects
- more realistic simulation of fish, by improving representation of respiration, consumption, spawning and elimination of toxicants
- enhanced output for nutrient analysis by computing chlorophyll *a* for periphyton, bryophytes, and phytoplankton, and computing the limitation factors for photosynthesis
- increased number of organic toxicants (up to 20) that can be modelled simultaneously enhanced uncertainty analysis capabilities.

AQUATOX is now an extension to BASINS (EPA's GIS-based watershed modelling system), providing linkages to geographic information system data, and output from BASINS' watershed models (HSPF and SWAT). Following errors were detected in release 1 and 1.1 and corrected in release 2.:

- a change in the bathymetric computations affecting the areas of the thermocline and littoral zone
- removal of an unnecessary conversion from phosphate and nitrate, assuming that all nutrient input is in terms of N and P; this could affect nutrient limitations
- inclusion of an oxygen to organic matter conversion factor (a factor of 1.5) and inclusion of specific dynamic action in the allometric computation of fish respiration
- adding a conversion factor for wind measured at 10 m height to wind occurring at 10 cm above the water surface in the volatilization computations; for some compounds this could result in a two-fold reduction in volatilization
- nitrification is formulated to occur only at the sediment-water interface bioaccumulation, and hence toxicity, are constrained by the life span of an animal.

Assumptions and Limitations:

The aquatic system is assumed well mixed (point model) but stratification can be taken into account.

Model Validation Reports:

The following validation reports are from Release 1 and 1.1. They have not been re-done using the Release 2 code, so the model results would be somewhat different. But the overall results and conclusions should still be valid.

Download of nutrient analysis on the Onondaga Lake, New York

Download of nutrient analysis of the Coralville Reservoir, Iowa

Download of bioaccumulation of PCBs in Lake Ontario

Website:

http://www.epa.gov/waterscience/models/aquatox/

AusRivAS Australian RIVer Assessment System

Description:
AUSRIVAS is a prediction system used to assess the biological health of Australian rivers. AUSRIVAS was developed under the National River Health Program (NRHP) by the Federal Government in 1994, in response to growing concern in Australia for maintaining ecological values. The NRHP involves the major environmental agency in each state and territory and is centrally administered by Environment Australia (EA) and the Land and Water Resources Research and Development Corporation (LWRRDC). The AUSRIVAS predictive software was developed at the Co-operative Research Centre for Freshwater Ecology (CRCFE). Fundamental to AUSRIVAS are predictive models, based on the British RIVPACS models (**R**iver **I**n**V**ertebrate **P**rediction **A**nd **C**lassification **S**ystem, Wright, 1995). These models predict the aquatic macroinvertebrate fauna expected to occur at a site in the absence of environmental stress, such as pollution or habitat degradation, to which the fauna collected at a site can be compared. Thus, AUSRIVAS produces a biological assessment that can be used to indicate the overall ecological health of the site. AUSRIVAS macroinvertebrate predictive models have been developed for each state and territory for the main habitat types found in Australian river systems, including riffle, edge, pool and bed habitats. Each state/territory has models constructed from single season data in addition to models with data combined from several seasons. The AUSRIVAS predictive system and associated sampling methods offer a number of advantages over traditional assessment techniques. The sampling methods are rapid and standardised within each state/territory, fast turn around of results is possible and the outputs from the AUSRIVAS models are tailored for a range of users including community groups, managers and ecologists.

Data Requirement:
To use the AUSRIVAS models to assess test sites, the sampling must be performed in strict accordance with the specific state or territory protocol outlined in the appropriate sampling manual. The test sites must be sampled in a season, or seasons, that correspond with the reference site sampling used to construct the model. For example, if a riffle habitat spring/autumn model is used, riffle samples from the test site are collected in spring and autumn. Each of the predictor variables measured at a site has a standardised code which is used for data entry to allow the model to recognise and order that variable. The habitat variable codes required for each model can be viewed in the AUSRIVAS programme, as described in the "Preparing Data" section of the predictive modelling software user manual.

Output:
Group probabilities sheet

Family probabilities sheet

Predicted/collected sheet

Version and System Requirements:
Version 3.1.1

Application History:
Is increasingly incorporated into Australian State monitoring protocols.

Availability:
AusRivAS models can be downloaded from the Internet at the AUSVIRAS homepage.

Website:

http://ausrivas.canberra.edu.au/

BASINS **Better Assessment Science INtegrating Point and Nonpoint Sources**

Description:
Basin is a system developed by the USEPA to meet the needs of pollution control agencies in the U.S. It integrates a geographic information system (GIS), national catchment data and state-of-the-art environmental assessment and modelling tool into one package. The heart of BASIN is its suite of interrelated components essential for performing catchment and water quality analysis. These components are grouped into five categories. (1) National databases. (2) Assessment tools (TARGET, ASSESS and Data Mining) for evaluating water quality and point sources loadings at a variety of scales. (3) Utilities including local data import, land-use and DEM reclassification, catchment delineation, and management of water quality observation data. (4) Catchment and water quality models including NPSM, TOXIROUTE and QUAL2E. (5) Post-processing output tools for interpreting model results.

Data Requirement and Data Output:
BASIN includes a post-processing tool to facilitate the evaluation and analysis of the model output. The graphical interface allows the user to select data sets, parameters, and locations; define output scales; and overlay multiple graphs and managements scenarios.

Version and System Requirements:
Minimum requirement is a 133-MHz Pentium processor and 32 Mb of RAM plus 32, but preferably a 200-MHz Pentium processor and 64 Mb of RAM plus 64 Mb of permanent virtual memory swap space. The 24X reader is preferred to the Quad speed reader. The operating systems are Windows 95, Windows 98 and NT*. Arc View, Version 3.0a, Arc View Dialog Designer or Arc View, version 3.1. In BASINS 3.0, in order to run the SWAT model or the automatic watershed delineator, ArcView requires the Spatial Analyst extension software. This software is not included with ArcView and must be purchased separately.

The USEPA and ESRI have entered into an agreement whereby nonprofit organisations (e.g. Federal, State, Tribal, or watershed groups developing TMDLs) may obtain Spatial Analyst version 1.1 at a reduced price. For those who are interested send name, address, and phone number to mailto:kinerson.russell@epa.gov to obtain a copy.

Application History:
Beside BASINS' primary role in creating TMDL analysis, it has been useful in identifying impaired surface waters from point and nonpoint pollution, wet weather combined sewer overflows (CSO), storm water management issues, and drinking water source protection. BASINS has also been used in urban/rural landuse evaluations, animal feeding operations, and habitat management practices. Another unexpected use of BASINS is providing schools and educational institutions with a quick, free resource of GIS and surface water data for the United States

Availability:
For more information on content, availability, and training, please contact:

Standards and Health Protection Division (4305T)

Office of Science and Technology

Office of Water

U.S. Environmental Protection Agency

1200 Pennsylvania Avenue, NW, Washington, DC 20460

Fax:202-566-0409

BASINS email: basins@epa.gov

Website:

http://www.epa.gov/waterscience/basins/basinsv3.htm

BATHTUB

Description:
Applies a series of empirical eutrophication models to morphologically complex lakes and reservoirs. The programme performs steady-state water and nutrient balance calculations in a spatially segmented hydraulic network which accounts for advective and diffusive transport, and nutrient sedimentation. Eutrophication-related water quality conditions (total phosphorus, total nitrogen, chlorophyll-*a*, transparency, and hypolimnetic oxygen depletion) are predicted using empirical relationships derived from assessments of reservoir data (Walker, 1985).
BATHTUB can be interrelated with the programmes PROFILE and FLUX to simplify assessments of eutrophication-related processes and effects.

Data Requirement:
BATHTUB requires information describing watershed characteristics, water and nutrient loads, and lake or reservoir morphology. Observed lake or reservoir water quality data are desirable. FLUX can deliver mass loads, and associated error statistics (CV) as input to BATHTUB. PROFILE can deliver mixed-layer water quality summaries (means) and hypolimnetic oxygen depletion rates, and associated error statistics (CV) as input to BATHTUB.

Output:
Model outputs include tabular and/or graphic displays of segment hydraulics, water and nutrient balances, predictions of nutrient concentrations, transparency, chlorophyll-*a* concentrations, and oxygen depletion. Statistics relating observed and predicted values are provided.

Version and System Requirements:
MS DOS; PC Compatible.

Assumptions and Limitations:
Applications of BATHTUB are limited to steady-state evaluations of relations between nutrient loading, transparency and hydrology, and eutrophication responses. Short-term responses and effects related to structural modifications or responses to variables other than nutrients can not be explicitly evaluated.

Application History:
The programmes and models have been applied to US Army Corps of Engineer reservoirs (Kennedy, 1995), as well as a number of other lakes and reservoirs.

Availability:
Distributor: Dr. Robert H. Kennedy

Environmental Laboratory

U.S. Army Engineer Waterways Experiment Station

3909 Halls Ferry Road

Vicksburg, MS 39180

Email: kennedr@wes.army.mil

Website:

http://www.wes.army.mil/el/elmodels/emiinfo.html

BEAST	**BEnthic Assessment of Sediment**

Description:
BEAST software was developed to provide an alternative to current guidelines and criteria. It employs both environmental and biological factors, and allows appropriate site-specific biological objectives to be set for ecosystems. These objectives are established using measured habitat characteristics and provide a reference point for determining when degradation is occurring at a site.

The core of the BEAST system is the reference condition database, which provides comparative environmental and community structure data for uncontaminated or ‘clean’ sites. Reference data are then combined with test (contaminated) data provided by the user, through the use of multivariate statistical analysis to assess sediment contamination. Reference databases for the Great Lakes and Fraser River are available. Reference databases can also be developed independently by users of the BEAST, although such an undertaking involves a much more significant investment of time, materials, and effort (Reynoldson *et al*., 2000).

Output:
BEAST produces ordination ellipses -- graphs showing the relationship between test sites and reference sites matched by habitat attributes. Overall stress at a test site is determined by its worst position in ordination space, on all vectors of the ordination. Toxicity tests performed on test sediment samples can also be analysed and displayed using two methods. The first - ordination - produces an ellipse plot. The second involves a bio-assay endpoint scoring system developed in conjunction with BEAST. Endpoint scores for each of the acute and chronic toxicity organisms are graphed for each test site. The level of impact for each site in a particular test is determined according to the number of standard deviations away from the mean of the endpoint score. Summary impact results for a test site are displayed in graphic and tabular form, using the results for all ten endpoint scores. Site maps can be produced by the BEAST to display both reference and test sites. Test sites can be mapped according to predictive grouping, and impact analysis (both community and toxicity impact).

Application History:
Used as record tool.

Website:

http://www.ec.gc.ca/ceqg-rcqe/English/Html/SAS/factsheet_3.cfm

BMWP **Biological Monitoring Working Party System**

Description:

The BMWP System was set up by the Department of the Environment to recommend a biological classification system for use in national river pollution surveys. It first met in March 1976 with the following terms of reference:

* To recommend a biological classification of river water quality for use in river pollution surveys;
* To consider ways and means of implementation;
* To consider relationships, if any, between chemical and biological classifications.

The Working Party initially decided not to correlate the chemical and biological assessments, and after many meetings and much discussion, the Interim Report of the BMWP was published by the Department of the Environment in 1976. This recommended, by a majority decision, the development of a score system based on the benthic macro-invertebrates. Trial use of this recommended methods by the water industry led to major changes in the proposed procedures prior to the presentation of the Final Report in 1978. These changes involved:

* Reduction in the level of taxonomic identification required;
* Removal of the proposed fauna abundance ratings;
* Reduction of river types to only eroding or depositing habitat types;
* Acceptance of a lack of a standardised sampling procedure;
* Allocation of family scores based on their most pollution tolerant species.

In the Final Report separate scores were allocated for eroding and depositing zones. They ranged from one for pollution tolerant Oligochaeta (worms), up to 100 for the most pollution sensitive families. It was fortuitous that this Final Report was never officially published, since, after further trials by the water industry, yet more changes were made prior to the use of the system for National River Surveys. These involved:

* Combining the eroding and depositing habitat types into a single type;
* Reducing the family scores to a range of one to ten to minimise the final score.

A weakness of the BMWP system, in common with many other score systems, is the effect of sampling effort. A prolonged sampling period can be expected, under most circumstance, to produce a higher final score than a sample taken quickly. To overcome this inherent weakness of the BMWP system, it became common practice to calculate the Average Score Per Taxa (ASPT) by dividing the BMWP Score by the number of taxa. The inclusion of the ASPT in reporting the 1990 National Biological Survey made possible the reappraisal of scores carried out by Walley and Hawkes (1996, 1997). This work showed the significant effects the site type had on the score, thus reinforcing the original BMWP's use of different scores for eroding and depositing substrates.

Website:

http://lakes.chebucto.org/ZOOBENTH/biotic.html - BMWP

CatchMOD	Catchment Modelling Cluster

Description:
Within the EU's 5th Framework Programme a variety of RTD projects have been funded which are clustered in the Catchment Modelling cluster. The projects cover a wide range of subjects, dealing with specific issues in water management, in international co-operation and collaborative planning, modelling methodologies and ICT tools. The objectives of clustering are to exchange information, discuss and solve common problems, make use of each others intermediate products and expertise: reach beyond the limited possibilities of isolated projects. Besides obvious collaboration on specific water and modelling issues, exchange of experience and approaches to end-user involvement, stakeholder participation and socio-economic issues are crosscutting themes for many of the CatchMod projects. The concerted action Harmonised Modelling Tools for Integrated Basin Management, Harmoni-CA will fulfil a central role within the CatchMod Cluster. The objective is to create a forum for unambiguous communication, information exchange and harmonisation of the use and development of ICT-tools1 relevant to integrated river basin management, and the implementation of the WFD. The communication, information exchange and harmonisation is geared towards the development of a widely accepted, flexible, harmonised modelling toolbox, including ICT-tools, guidance and methodologies, which can be applied by the various stakeholders in river basins. Amongst these stakeholders are end-users of models and tools as well as basin planners, policy developers, the public etc.

Catchmod Cluster Projects:

HarmoniQuA,; Euroharp; HarmoniRiB; BMW; Tisza River Project; Daufin; EuroLakes; FIRMA; Gouverne; HarmoniCA; HarmoniCoP; Mulino; TempQSim; Transcat and Clime.

Website:

http://www.harmonit.org/links/catchmod.htm

CATS-5 — *C*ontaminant in *A*quatic and *T*errestrial eco*S*ystems

Description:

CATS-5 has been constructed to model the combined effects of micropollutants and nutrients in aquatic systems. An existing eutrophication module (Janse *et al*., 1992 and Janse, 1996) was combined with a fate module from SIMPLEBOX, an existing food-web of micropollutants (Traas *et al*., 1995; 1996) and an effects module (Traas *et al*., 1998; 2001).

Assumptions and Limitations:

The aquatic system is assumed well mixed (point model) and average daily conditions are modelled. Equilibrium partitioning of pesticides among the organic phases is assumed, except for sediment where diffusion-limited exchanges between water and pore water is taken into account. Mortality of invertebrates, algae and macrophytes is based on the toxicant concentration in the water.

CATS-5 is not applicable to hydrophobic toxic compounds that show significant association with biotic particles and are readily taken up in the food chain. Trophic transfer is not included into the model. Additional toxicity by contaminants uptake by food or bioconcentration is not simulated.

Application History:

Simulations were tested against chlorpyrifos data collected in aquatic microcosm experiments CATS-5 reproduced the observed effects of nutrients, chlorpyrifos and their interaction reasonably well (Janse and Traas, 1996). .

CE-QUAL-W2 A hydrodynamic and water quality model for rivers, estuaries, lakes, and reservoirs

Description:

CE-QUAL-W2 is a two-dimensional, laterally averaged, finite difference hydrodynamic and water quality model. Because the model assumes lateral homogeneity, it is best suited for relatively long and narrow water bodies exhibiting longitudinal and vertical water quality gradients. The model can be applied to rivers, lakes, reservoirs, and estuaries. Branched networks can be modelled. The model accommodates variable grid spacing (segment length and layer thickness) so that greater resolution in the grid can be specified where needed. The model equations are based on the hydrostatic approximation (negligible vertical accelerations). Eddy coefficients are used to model turbulence. The hydrodynamic time step is calculated internally as the maximum allowable time step that ensures numerical stability. A third-order accurate (QUICKEST) advection scheme reduces numerical diffusion. The water quality portion of the model includes the major processes of eutrophication kinetics and a single algal compartment. The bottom sediment compartment stores settled particles, releases nutrients to the water column, and exerts sediment oxygen demand based on user-supplied fluxes; a full sediment diagenesis model is under development.

Data Requirement:

The application of CE-QUAL-W2 requires knowledge in the following areas:

- Hydrodynamics
- Aquatic biology
- Aquatic chemistry
- Numerical methods
- Computers and FORTRAN coding
- Statistics
- Data assembly and reconstruction

Output:
The model allows the user considerable flexibility in the type and frequency of outputs. Output is available for the screen, hard copy, plotting, and restarts. The user can specify what is output, when during the simulation output is to begin, and the output frequency. The present version requires the user to develop output plotting/visualization capabilities. Version 3.0 will include graphical pre- and postprocessors for plotting/ visualization

Version and System Requirements:
The minimum configuration is an 80386 PC equipped with a math coprocessor. A minimum of four megabytes of memory is needed unless the user has an operating system or extender that uses virtual memory. A hard disk with a minimum available space of 25 MB is also required.

Assumptions and Limitations:
Well-mixed in lateral direction (but can be used in a Quasi-3-D mode by use of additional model branches), hydrostatic assumption for vertical momentum equation

Application History:
Widespread use in US, in particular for more complicated scenarios associated with protocols for TMDLs.

Availability:
Distributor: Thomas M. Cole

Environmental Laboratory

U.S. Army Engineer Waterways Experiment Station

3909 Halls Ferry Road

Vicksburg, MS 39180

mailto:tcole@lasher.wes.army.mil

Website:

http://www.wes.army.mil/el/elmodels/w2info.html

CORINE Co-ORdination of INformation on the Environment

Description:

Programme Objectives CORINE was established in June 1985 by the European Community's Council of Ministers. It was given three main objectives:

1) to gather information on the state of the environment, for use in priority Community applications; 2) to coordinate national initiatives taken by Member States, and to improve information at the international level; and 3) to ensure the consistency of nomenclatures, definitions, etc., as well as creating the conditions necessary to compare data.

All three objectives were intentionally seen as interdependent. Within this framework, there were defined a number of priority areas, including the protection of biotopes, combating local and transboundary air pollution and to preserve the environment of the Mediterranean region. *Type of Programme:* Intergovernmental; Data and Information Management; Coordination. *Data and Information Management:* The CORINE Information System has three components:

1. projects (air pollution, biotopes, coastal erosion, land cover, marine environment, soil erosion/quality, and water resources;
2. data collected under EC Legislation; and
3. basic data required for analysis and presentation of results.

These components aim to provide the information requirements of the objectives. The associated data sets and information have been organized within two broad areas:

1. the compilation of environmental data and the development of a Geographical Information System (GIS) on the state of the environment in Europe; and
2. the improvement of consistency, comparability, and availability of environmental data. This is to be addressed by developing standards for the collection, handling and management of environmental data. The essential component of this system is its integration. In other words, information from various sources must be made intercompatible. The ARC/INFO system contains modules which will allow the conversion between commonly used projections. Once fully developed, this system will be similar in nature to UNEP's Global Resource Information Database

Availability:

Commission of the European communities

Environment, Nuclear Safety and Civil

Protection - Agency Task Force DG XI

Rue de la LOI 200

B-1049 BRUSSELS, BELGIUM

Telefax: +32 02 235 01 44

Website:

http://www.eea.eu.int//

CORMIX **CORnell MIXing zone model**

Description:
This is the Cornell University mixing zone model, it was developed primarily to analyse the near-field problem. This model consists of a series of software subsystems for the analysis, prediction and design of aqueous toxic or conventional pollutant discharges into diverse water bodies. The system's primary emphasis is on predicting the geometry and dilution characteristics of the initial mixing zone so that compliance with acute and chronic regulatory constraints may be assessed; the system also predicts the behaviour of the discharge plume at greater distance

Output:
Near field and far field plume trajectory, shape, concentration and profile. Dilution predictions, density current predictions

Version and System Requirements:
The hydrodynamic models of CORMIX v3.2 (DOS) have been extensively updated in CORMIX v4.2.

Assumptions and Limitations:
In tidal situations, CORMIX only considers the plume behaviour within the immediate tidal cycle and has no information about the thermal history which may exist in the real environment from preceding tidal cycles. CORMIX also idealizes the physical configuration of the receiving water and solves for a straight shoreline. Problems simulating effluent plumes during near-slack (i.e., low ambient current) conditions. Problems simulating effluent plumes from outfalls located in shallow waters. Inability to simulate effluent plumes from surface discharge pipes over a full range of tidal conditions. The flow solutions used by CORMIX depend on assuming that the discharge is from a well-defined channel of specified depth or a fully submerged pipe.

Application History:

CORMIX predicts mixing behaviour from diverse discharge types ranging from power plant cooling waters, desalinisation facility or drilling rig brines, municipal wastewater, or thermal atmospheric plumes. CORMIX has been applied across a broad range of ambient conditions ranging from estuaries, deep oceans, swift shallow rivers, to density stratified reservoirs and lakes.

Availability:

Dr. Russell Kinerson at the Office of Science and Technology (OST) is the primary contact for CORMIX support services. The Oregon Graduate Institute of Science and Technology (OGI), under a cooperative agreement with EPA, provides CORMIX information, distribution, and technical support services to the CORMIX user community. The CORMIX home page contains updated information about software releases, model applications, and tools for regulatory mixing zone decision support. The P. I. for the OGI/OST cooperative agreement is Dr. Robert L. Doneker (503) 748-4053 at the Department of Environmental Science and Engineering, Oregon Graduate Institute.

Cormix can be downloaded from the WWW at:

http://asellus.cee.odu.edu/model/cormix.php

Website:

http://www.cormix.info/

CREAMS **Chemicals, Runoff, and Erosion from Agricultural Management Systems**

GLEAMS **Groundwater Loading Effects of Agricultural Management Systems**

Description:

Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS) was developed by the U.S. Department of Agriculture—Agricultural Research Service (Knisel, 1980; Leonard and Ferreira, 1985) for the analysis of agricultural best management practices for pollution control. CREAMS is a field scale model that uses separate hydrology, erosion, and chemistry submodels connected together by pass files. Runoff volume, peak flow, infiltration, evapotranspiration, soil water content, and percolation are computed on a daily basis. If detailed precipitation data are available then infiltration is calculated at histogram breakpoints. Daily erosion and sediment yield, including particle size distribution, are estimated at the edge of the field. Plant nutrients and pesticides are simulated and storm load and average concentrations of sediment-associated and dissolved chemicals are determined in the runoff, sediment, and percolation through the root zone (Leonard and Knisel, 1984). User defined management activities can be simulated by CREAMS. These activities include aerial spraying (foliar or soil directed) or soil incorporation of pesticides, animal waste management, and agricultural best management practices (minimum tillage, terracing, etc.). Calibration is not specifically required for CREAMS simulation, but is usually desirable. The model provides accurate representation of the various soil processes. Most of the CREAMS parameter values are physically measurable. The model has the capability of simulating 20 pesticides at one time. Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) was developed by the United States Department of Agriculture—Agriculture Research Service (Leonard *et al*., 1987) to utilize the management oriented physically based CREAMS model (Knisel, 1980) and incorporate a component for vertical flux of pesticides in the root zone. A nitrogen component for the root zone is in development.

GLEAMS consists of three major components namely hydrology, erosion/sediment yield, and pesticides. Precipitation is partitioned between surface runoff and infiltration and water balance computations are done on a daily basis. Surface runoff is estimated using the Soil Conservation Service Curve Number Method as modified by Williams and Nicks (1982). The soil is divided into various layers, with a minimum of 3 and a maximum of 12 layers of variable thickness are used for water and pesticide routing (Knisel *et al*., 1989).

Data Requirement:

The data needed for CREAMS are quite detailed. As CREAMS is a continuous simulation model the data needs are extensive. Meteorological data consisting of daily or breakpoint precipitation is required for hydrology simulation. Monthly solar radiation and air temperature data is also needed for estimating components of the hydrological cycle. Data regarding soil type and properties along with information on crops to be grown is needed. A broad range of values for various model parameters can be obtained from the users manual.

Output:

Various output options are available for hydrology and nutrient simulations, including storm, monthly, or annual summary. Output for each segment of the overland flow and channel elements is available from areas in the watershed where intense erosion or deposition can be identified.

Version and System Requirements:

The maximum size of the simulated area is limited to a field plots. A watershed scale version (Opus) of CREAMS/ GLEAMS is currently under development. The model is limited in data management and handling. The model cannot simulate instream processes. Although CREAMS has been applied in a wide range of climatic regimes, there is concern regarding its simulation capability for snow accumulation, melt, and resulting runoff, and hydrologic impacts of frozen ground conditions (Knisel *et al*., 1983).

Assumptions and Limitations:

The programme is written in standard FORTRAN 77 and has been installed on IBM PC/AT-compatibles. A hard disk is required for operation of the program and a math co-processor is highly recommended. The programme can be obtained on floppy disk for MS/DOS operating systems.

Application History:

CREAMS has been extensively applied in a wide variety of hydrologic settings with good success. CREAMS has been used for in a wide variety of hydrologic and water quality studies (Smith and Williams, 1980; Lane and Ferreira, 1980 and Knisel *et al*., 1983). Crowder *et al.* (1985) have used CREAMS in conjunction with an economic model to evaluate effects of conservation practices.

Availability:

To obtain copies of the model please write or call Dr. Walt Knisel or Frank Davis at the following address:

USDA-Agricultural Research Service

Southeast Watershed Research Lab

P.O. Box 946

Tifton, Georgia 31793

(912) 386-3462

Website:

CREAMS:

http://dino.wiz.uni-kassel.de/model_db/mdb/creams.html

GLEAMS:

http://www.ars.usda.gov/research/publications/publications.htm?SEQ_NO_115=104920

DAISY	Soil-plant system model

Description:
Model for the simulation of soil water and nitrogen dynamics in the crop-soil system. The main modules simulate: water dynamics, including snow accumulation and melting, evaporation from open water surfaces and soil, transpiration and water uptake by plants (based on the single root uptake and root density), infiltration, percolation and soil water dynamics (Richard's equation); soil heat, including freezing and melting and soil temperature; nitrogen dynamics, including turnover of organic matter (based on carbon pools, microbial biomass, and first order kinetics), mineralisation/immobilization (a consequence of the carbon turnover), nitrification, denitrification, nitrogen uptake by plants (based on single root uptake and root density), and nitrogen transport (convection-dispersion equation) and leaching; crop growth, i.e. crop development, dry matter production, crop nitrogen demand, crop nitrogen content, photosynthesis, water stress, nitrogen stress, assimilate partitioning, maintenance and growth respiration, leaf area development, root penetration and root density distribution. The model allows for the simulation of different management strategies and crop rotations.

Data Requirement and Output:
In a first step DAISY_1 solves the models for soil water dynamics, soil heat and crop production limited by radiation and soil water content only. It requires information about physical soil layers (soil hydraulic and thermal properties), numerical soil layers (user defined node points), initial and boundary conditions (for the bottom boundary either a Neuman or a Dirichlet condition can be defined), crop, tillage, management, weather data for precipitation, air temperature, potential evapotranspiration and (optionally) groundwater table depth on a daily basis.

The output (water content, ice content, plant-water-uptake, temperature and flux density versus time and depth) is stored in binary format on disc. This allows simulations over several years while maintaining an hourly time step for the calculated fluxes. DAISY1 produces 2.5 Mbyte/year output.

In a second step, DAISY_2 uses the output of DAISY_1 as input. It calculates carbon turnover, microbial biomass-dynamics, solute-dynamics, and nitrogen limited crop production. Output is given on a daily basis, resulting in 0.5 MByte/Year. Daisy2 requires initialisation of the chemical and biological processes and several parameters describing the transformation characteristics the soil. These include laboratory determined rate constants for nitrification and denitrification, impendance factors, longitudinal dispersivity, NH4-adsorption -isotherm, average dry and wet nitrogen deposition rates/concentrations. The total soil organic matter is divided into four fractions dependent upon history and origin. A fraction is further divided into two pools with fast and slow turnover rates. Each of the four main organic matter fractions is specified by a minimum of seven constants. Some of the required parameters may be difficult to access experimentally. The authors provide default values and examples of initialisation files worked out for agricultural crops in humid north-west European climate.

Version and System Requirements:
Operating System(s): DOS, numeric coprocessor required The following executables are available from the Authors upon request: daisy1.exe: calculates soil water and soil temperature dynamics; daisy2.exe: carbon - and nitrogen dynamics, using binary hourly output data provided by daisy1; sp-daisy.exe: utility program, estimates soil hydraulic and thermal functions from measured data, creates soil hydraulic and thermal properties arrays used by daisy1 utilities to convert the binary output files of daisy 1 (water/ice content, temperature and flux density versus time and depth) to ASCII- files

Assumptions and Limitations:
Specific climate, soil hydraulic conditions and soil thermal properties may be defined in the input files. Crop parameters are only defined for spring barley, rye grass, winter wheat, rape

Availability:

Contact:

Soeren Hansen

The Royal Veterinary and Agricultural University

Department of Agricultural Sciences, Agrohydrology

Thorvaldsvej 40

DK-1871 Fredriksberg C

Denmark

Phone: +45 35 28 33 86

Fax : +45 35 28 33 84

Email: soeren.hansen@agsci.kvl.dk

Website:

http://www.dina.kvl.dk/~daisy/

DATBAL

Description:
DATBAL is a screen routine that prompts the user for keyboard entry and automatically creates a file in SCOR format. It also can be used to edit existing SCOR data files and to balance automatically any network so that the inputs and outputs associated with each system component are equal. Can be used with other routines e.g. NTWRK.

Availability and Website:
The programme is available as a download at:

http://www.cbl.cees.edu/~ulan/ntwk/network.html

DHRAM **Dundee Hydrological Regime Assessment Method**

Description:
The Water Framework Directive (WFD) of the European Union is the principal driver behind the development of protocols for the assessment of anthropogenic impacts on the hydrology of Scotland's rivers, lakes and transitional waters. A new approach for rivers, known as the Dundee Hydrological Regime Assessment Method (DHRAM) has been developed. The underlying rationale is to assess the risk of significant impact on biota arising from changes in hydrological regime, as distinct from chemical or hydromorphological influences. This approach is based on the Indicators of Hydrologic Alteration (IHA) methodology of Richter *et al.* (1996), in which the degree of alteration of a range of hydrological variables that are significant to biota are estimated. The DHRAM method classifies the degree of alteration to hydrological regime using a five-point scale, which correlates with the risk of ecological damage. These categories are compatible with those of the WFD. The acquisition of appropriate biological data for calibration and validation of DHRAM has, however, proved problematic. This paper proposes the future development of a calibration scheme which compares the biota of neighbouring water bodies (pairs whose physical attributes are as similar as possible in all relevant respects, except in the degree of disturbance to their hydrological regimes).

Data Requirement:
Daily mean river flows in un-impacted and impacted conditions for the site of interest, preferably 20 years comparable data. Synthetic data may be used. For lakes, daily level data are required – other requirements as for rivers.

Output:
32 Indicators of hydrologic alteration; final alteration classification on 1-5 scale

Version and System Requirements:
Code exists in unix and Windows versions

Assumptions and Limitations:
Input data assumed to be reliable (an important assumption if using modelled data). Thresholds used in determining severity classification are appropriate to Scotland only; an empirical study for Ireland would help for application.

Application History:
Unix version developed for University of Dundee use only. Windows version developed under contract to Scottish Environment Protection Agency. Requires enhancement to user interface.

Availability:
A Windows version may be available on application to the author

Website:

None. Enquiries: Dr Andrew Black, University of Dundee,

mailto:a.z.black@dundee.ac.uk

DIVAST Depth Integrated Velocity And Solute Transport

Description:
Typically DIVAST (TRIVAST in three dimensions) is used for predicting flow, water quality and sediment transport processes in coastal, estuarine and inland waters. A 2D depth integrated, hydrodynamic and water quality model. The model solves the conservation equations of mass, momentum and solute and sediment transport. Sub modules: Hydrodynamic, Sediment Transport, Heavy Metals, Solute Transport and Water Quality. The model accurately represents flooding and drying of mudflats during flood and ebb tides.

Data Requirement:
Boundary hydrodynamics, riverine / marine fluxes, parameter-specific characteristics.

Output:
Concentrations / values of each variable including the parameters

- dissolved oxygen
- Biochemical oxygen demand
- nitrogen (organic and inorganic)
- phosphorous (organic and inorganic)
- silicate
- chlorophyll_*a*
- diatoms
- Salinity
- Temperature
- Suspended solids (cohesive and non-cohesive)
- Coliforms
- Heavy metal:- lead, zinc, mercury, cadmium

User-defined pollutant (first-order reaction)

Assumptions and Limitations:
Complete vertical mixing.

Application History:
The model has been developed by Professor Falconer (University of Cardiff) specifically for application in estuarine and coastal waters. Within the Irish Sea, the models have been set-up for many locations, including the Mersey Estuary to predict the fate of priority organic and metal pollutants, the prediction of velocities and faecal coliform distributions have been undertaken at Morecambe Bay, within the Bristol Channel and along the Fylde Coast and Ribble Estuary. The model has been widely applied in Ireland for water quality analysis, for example it has been applied to Donegal Bay, Cork Harbour and Wexford Harbour. Recently the MarGIS package has incorporated DIVAST into ArcView 8, allowing model creation, editing and execution be performed within MarGIS. This tool allows model results visualisation either as time history graphs, plume shots or animations of two-dimensional plumes throughout an estuary.

Availability:
Prof. Roger Falconer, Cardiff University.

Email: FalconerRA@cf.ac.uk

Environmental Water Management Research Centre

Cardiff School of Engineering

Cardiff University

PO Box 925

Cardiff CF24 0YF

Wales UK

MarGIS is available from MarCon Computations International Ltd., Galway.

Website:

http://www.engin.cf.ac.uk/research/summary.asp?GroupNo=3

DRAINMOD **Methods for Design and Evaluation of Drainage-Water Management Systems for Soils with High Water Tables**

Description:
DRAINMOD simulates the hydrology of poorly drained, high water table soils on an hour-by-hour, day-by-day basis for long periods of climatological record (e.g. 40 years). The model predicts the effects of drainage and associated water management practices on water table depths, the soil water regime and crop yields. It has been used to analyse the hydrology of certain types of wetlands and to determine whether the wetland hydrologic criterion is satisfied for drained or partially drained sites. The model is also used to determine the hydraulic capacity of systems for land treatment of wastewater.

Data Requirement:
* General information
* Weather inputs
* Drainage design parameters
* Lateral saturated hydraulic conductivity
* Soils data
* Traffic ability inputs
* General crop inputs
* Sprinkler (waste) irrigation
* Crop yield parameters and crop data
* Wetland hydrology determinations

Output:
Outputs from the model can be easily imported in other applications such as spreadsheets for analysis. The latest version includes some graphic analysis of the model results. There are a number of output options. Daily, monthly and annual summaries include infiltration, evapotranspiration, depth to the water table, runoff, drainage volume, number of work days based on soil air volume, drought and wet stresses. The model also produces an annual ranking for computing recurrence intervals for many of the outputs.

Version and System Requirements:
The latest version, DRAINMOD Ver 5.1 combines the original DRAINMOD hydrology model with DRAINMOD-N (nitrogen sub-model) and DRAINMOD-S (salinity sub-model) into a Windows based programme. The new version includes a graphical user interface that allows easy preparation of input data sets, running simulations as well as displaying model outputs. In addition to organizing the hydrology, nitrogen, and salinity components of DRAINMOD, the interface facilitates analyses of the effect of drainage system design on subsurface drainage, surface runoff, SEW30, crop yield, and nitrogen loss in surface and subsurface drainage by automatically editing drainage design parameters (e.g. drain spacing & drain depth) over a specified range, simulating the different designs and graphically displaying the results. The interface also calculates the runoff volume from surrounding areas that drain to a site and adds that runoff volume to a DRAINMOD water balance of the site. Version 5.1 also includes routines for soil temperature modelling and considers freezing and thawing effects on drainage processes.
DRAINMOD-N (Breve, 1994) - DRAINMOD based field scale model for predicting Nitrogen from agricultural lands.

Assumptions and Limitations:
Snow, snowmelt and frozen ground runoff are not considered. The model can not be applied directly to sites that receive overland flow.

Application History:
DRAINMOD was first distributed by NRCS (formerly SCS) in the late 1970's as tool to assist state and regional engineers in developing water management system designs. Since this time, other users have also been using the model. The users include other researchers and modellers, consulting firms, and various state and federal agencies. Prior to the initial release to NRCS, the model was field tested in North Carolina (Skaggs, 1982). Through both cooperative and independent efforts, the model has been subsequently tested in many parts of the world.

Additionally, nitrogen and salinity portions of the model have been tested by Breve *et al*. (1997) and Kandil *et al*. (1995) and Merz and Skaggs (1998). Other field testing is currently on going for these versions of the model.

Availability:

The latest version of DRAINMOD (Version 5.1), the model is available for download. In order to install the model, please get a product key from Dr. Glenn Fernandez.

Email: gfernand@eos.ncsu.edu

Website:

http://www.bae.ncsu.edu/soil_water/drainmod/

DR3M-QUAL **Distributed Routing Rainfall Runoff Model—QUALity**

Description:

The Distributed Routing Rainfall Runoff Model—Quality (DR3M-QUAL) incorporates water quality routines into an updated version of an earlier U.S. Geological Survey (USGS) urban hydrologic model (Dawdy *et al.*, 1972). Runoff is generated from rainfall using the kinematic wave method over multiple sub-catchments and routed through drainage pathways by the same technique. Storage-indication routing is available for storage basins. The model can be run over any time period and is sometimes used to simulate a group of storms while bypassing simulation of the intervening dry periods (although a moisture balance is maintained). A built-in optimisation routine aids in estimation of quantity parameters. Quality is simulated for arbitrary parameters using exponential build-up functions plus wash-off functions determined from experience with model calibration. Considerable guidance is provided for parameter estimation. Removal of built-up solids can occur during dry weather by street cleaning. Erosion is simulated using empirical equations relating sediment yield to runoff volume and peak. Some guidance is provided for the erosion parameters using relationships based on the Universal Soil Loss Equation. Concentrations of other constituents can be taken as a fraction ("potency factors") of sediment concentration. Precipitation can contribute a constant concentration. Quality routing through the drainage network is done by a Lagrangian scheme to simulate plug flow and no decay. Plug flow routing is also performed in storage basins, with settling based on sedimentation theory and dependent on a particle size distribution.

Data Requirement:

Data needs depend on the degree of schematisation. Quantity parameters for a sub-catchment include area, imperviousness, length, slope, roughness and infiltration parameters. Channels are characterised by trapezoidal or circular dimensions and kinematic wave parameters. Storage basins require stage-area-discharge relationships. Quality parameters include build-up and wash-off coefficients. Rainfall input can be for single or multiple storms.

Quantity data are similar in form to those required by other urban hydrologic models and may be derived from contour maps and drainage plans available from municipalities. Build-up and wash-off parameters are very difficult to estimate a priori and require local, site-specific quality measurements for calibration if accurate quality predictions are needed, e.g., to drive a receiving water quality model.

Output:
DR3M-QUAL produces a time history of runoff hydrographs and quality pollutographs (concentration or load vs. time) at any location in the drainage system. Summaries for storm events are provided as well as line printer graphics for hydrographs and pollutographs.

Version and System Requirements:
The program is written in Fortran 77 for IBM or Prime mainframes. Source code is provided on a 9-track magnetic tape for compilation and installation on the user's computer.

Assumptions and Limitations:
The kinematic wave is perhaps as good a conceptual model as exists for overland flow but approximations are always inherent in its application, as for any conceptual model. The quantity model can be expected to perform reasonably well with minimal calibration. No interaction among quality parameters exists (other than the ability to treat one pollutant as a fraction of sediment concentration). Except for the sedimentation algorithm within storage units, simulation of sediment transport processes is weak, as with virtually all other models of this type. Generally, quality predictions must be calibrated if accurate concentrations and loads are required, e.g., to drive a receiving water quality model. On the other hand, relative comparisons can be made using generalized U.S. data for calibration purposes.

Application History:
The basis for the hydrologic components of DR3M-QUAL is the earlier modelling work of Dawdy *et al.* (1972) that was updated first for the quantity portion of the model (Dawdy *et al.*, 1978; Alley and Smith, 1982) and then for additional quality routines (Alley and Smith, 1982). Much of the emphasis on the form and calibration of build-up and wash-off parameters is based on research done by Alley and Smith (1981). The program has received extensive internal review within the USGS and has been applied to their urban modelling studies in South Florida (Doyle and Miller, 1980), Rochester (Kappel *et al.*, 1986; Zarriello, 1988), Denver (Lindner-Lunsford and Ellis, 1987), and Fresno (Guay and Smith, 1988). A summary of experience with the model is given by Alley (1986).

Availability:
The Fortran 77 source code and documentation are available on a 9-track magnetic tape (to be supplied by the user) from the USGS National Center):

Ms. Kate Flynn

U.S. Geological Survey

410 National Center

Reston, Virginia 22092

(703) 648-5313

Website:

http://water.usgs.gov/cgi-bin/man_wrdapp?dr3m

ECOHAM **Ecological North Sea Model Hamburg**

Description:
ECOHAM was originally developed (1994, as version ECOHAM0) for use on a main frame computer at the DKRZ in Hamburg, on a CRAY J90. Meanwhile the model system runs on a Personal Computer - Pentium III (450 MHz) and we call it version ECOHAM1. A simulation of the annual cycle of the year 1986 took 12 hours on such a machine. The downloads below include the FORTRAN code only, or the whole application for the North Sea including the model code and all necessary data files to run the simulation for 1986. The test case North Sea includes the forcing of the daily circulation data, the half hourly solar radiation data and the monthly river data to re-run the 1986 simulation and all additional initial and boundary data sets. The User Guide describes how to run the "model" with all necessary settings to reproduce the test case North Sea 1986. The ECOHAM model system is under development and we are working on version ECOHAM2 which will include the nitrogen cycle.

Data Requirement:
Initial and boundary conditions: long-term monthly mean nutrient concentration for several surface and bottom boxes (ERSEM boxes. Forcing functions: solar radiation every 30 minutes for each 1 x 1 box, circulation data every day (u, v, w, temperature, salinity, surface elevation, horizontal diffusion, vertical diffusion), river nutrient loads on a monthly basis for 14 rivers.

Output:
Variables: nutrient concentration (phosphate, dissolved inorganic nitrogen (DIN)), phytoplankton biomass (chlorophyll), sinking detritus, process rates (like primary production).
Formats: ascii data

Version and System Requirements:
CPU-time: 6 hours

Number of CPUs:1

Memory:256 MByte

Disk space: 800 MByte (Source code and input database)

Model output:Test configuration: 900 MByte (daily values)

Application History:
Research tool.

Availability:
Contact:

Dr. Andreas Moll

Institut für Meereskunde

Universität Hamburg

Troplowitzstr. 7

D-22529 Hamburg

Germany

Room: 106, I. Floor

Tel.: +49 (0)40 42838 2526

Fax.: +49 (0)40 560 57 24

moll@ifm.uni-hamburg.de

Download at:

http://www.ifm.uni-hamburg.de/~wwwem/dow/Ecoham/Model_Zip_Code_and_Data_Sets.html

Website:

http://www.ifm.uni-hamburg.de/~wwwem/dow/Ecoham/

ECOMSED **Estuarine and Coastal Ocean Model + SEDiment Transport**

Description:
ECOMSED is a three-dimensional hydrodynamic and sediment transport computer code developed by HydroQual for application to marine and freshwater systems. The component models are designed to execute in conjunction with each other so that output from one model is directly linked to the other models. The models share the same numerical grid structure and underlying numerical solution techniques. The development of ECOMSED has its origins in the mid-1980's with the creation of the Princeton Ocean Model followed by an upgraded version called ECOM for shallow water environments such as rivers, lakes, estuaries and coastal oceans. In the mid-1990s, concepts for sediment resuspension and settling developed by W. Lick at the University of California, Santa Barbara were incorporated within the ECOM modelling framework. Over the past several years, ECOMSED has been enhanced to include surface wave models, better bottom shear stresses for bottom boundary layer physics, non-cohesive sediment transport, and dissolved and sediment-bound tracer capabilities.

Data Requirement:
Sediment / particle characteristics, boundary hydrodynamics and fluxes.

Output:
Concentrations / values of each state variable.

Version and System Requirements:
ECOMSED can be run on UNIX platforms from all major vendors, the PC running LINUX, and PC running WINDOWS. The Make-files provided with the source code are for the UNIX/SGI and LINUX/INTEL operating systems. For the Windows platform, a suitable FORTRAN compiler should be used (it has been tested using Compaq Visual Fortran, release 6.1).

Assumptions and Limitations:
This model is more suited to deeper shelf waters than to coastal regions with sand banks and mudflats. Cannot deal with wetting and drying.

Application History:
ECOMSED simulates the transport and fate of suspended sediments, dissolved tracers and neutrally-buoyant particles in estuarine and coastal waters. Capabilities include:

- Runtime or pre-runtime computed hydrodynamics
- Cohesive and non-cohesive sediment transport
- Sediment-bound tracer transport (conservative or first-order decay)
- Dissolved tracer transport (conservative or first-order decay)
- Neutrally-buoyant particle tracking

Wind wave effects on hydrodynamics and sediment transport

Availability:
HydroQual, Inc.1 Lethbridge Plaza, Mahwah, New Jersey 07430.

ECOMSED is available for download to interested users by registering through HydroQual's website. HydroQual reserves the right to limit distribution of ECOMSED at its sole discretion.

Website:

http://www.hydroqual.com/Hydro/ecomsed/

ECOPATH

Description:
The parameterisation of an Ecopath model is based on satisfying two ‘master’ equations. The first equation describes the how the production term for each group can be divided:

Production = catch + predation + net migration + biomass accumulation + other mortality

It is the aim with the Ecopath model to describe all mortality factors; hence the ‘other mortality’ should only include generally minor factors as mortality due to old age, diseases, etc. The second ‘master’ equation is based on the principle of conservation of matter within a group:

Consumption = production + respiration + unassimilated food

The Ecopath software package can be used to

* Address ecological questions;
* Evaluate ecosystem effects of fishing;
* Explore management policy options;
* Evaluate impact and placement of marine protected areas;
* Evaluate effect of environmental changes.

Ecopath is a major element of EwE, an ecological software suite for PCs that has been under development for more than a decade. The development is centred at the University of British Columbia’s Fishery Centre, while applications are widespread throughout the world. The software has more than 2000 registered users representing 120 countries, more than a hundred ecosystem models applying the software have been published, see http://www.ecopath.org/. EwE has three main components: Ecopath, Ecosim and Ecospace.

Data Requirement:
Ecopath data requirements are relatively simple, and generally already available from stock assessment, ecological studies, or the literature: biomass estimates, total mortality estimates, consumption estimates, diet compositions, and fishery catches.

Output:
Energy and matter flux among defined ecological compartments, including losses through natural mortality and fishing.

Version and System Requirements:
It is presently being incorporated in Ecopath with Ecosim (EwE).

EwE has three main components: Ecopath – a static, mass-balanced snapshot of the system; Ecosim – a time dynamic simulation module for policy exploration; and Ecospace – a spatial and temporal dynamic module primarily designed for exploring impact and placement of protected areas.

Assumptions and Limitations:
Balances within the model make it susceptible to poor or low level data input.

Application History:
Used in many coastal situations, and multispecies fisheries (Christensen and Paul, 1993).

Availability and Website:
Ecopath and Ecosim are available for download after registration at: http://www.ecopath.org/

ECOSIM	**ECOsystem SIMulation**

Description:
Ecosim is a dynamic simulation module for predicting results of human and climatic impact on ecosystem components. Entering estimates of costs and prices allows the evaluation of bio-economic consequences of harvest strategies, while nonmarket valuation facilitates consideration of alternative uses of ecosystem resources. Ecosim also includes equilibrium analysis for predicting the impact of fishing effort on yield and biomass of all ecosystem components, and a routine for estimation of stock-recruitment relationships.

Version and System Requirements:
Ecosim was developed by Carl J. Walters of the Fisheries Centre, University of British Columbia, Vancouver. It is presently being incorporated in Ecopath with Ecosim (EwE).

EwE has three main components: Ecopath – a static, mass-balanced snapshot of the system; Ecosim – a time dynamic simulation module for policy exploration; and Ecospace – a spatial and temporal dynamic module primarily designed for exploring impact and placement of protected areas.

Availability:
A copy of Ecosim can be obtained at:

http://www.exetersoftware.com/cat/ecosim.html

Cost: $95. Multiple user license. Note: you may order any two of EcoSim, EcoStat, E-ZStat, or PopGene for $175, any three for $250, or all four for $300.

Or

It can be downloaded from the WWW at:

http://homepages.together.net/~gentsmin/ecosim.htm

Website:

http://www.isima.fr/ecosim/

EPIC — <u>E</u>rosion-<u>P</u>roductivity <u>I</u>mpact <u>C</u>alculator

Description:
EPIC is a mechanistic simulation model used to examine long-term effects of various components of soil erosion on crop production (Williams *et al*., 1984). Based on the conceptualisation of CREAMS, EPIC is a public domain model that has been used to examine the effects of soil erosion on crop production in over 60 different countries in Asia, South America and Europe. The model has a number of components which simulate, hydrology, soil erosion, plant growth dynamics, nutrient (N and P) cycling, soil temperature, economics, and crop management. EPIC added a number of components to the original CREAMS model, (i) a return flow component, (ii) reservoir storage component to predict the effects of farm ponds etc., a peak runoff rate calculation (based on a modification of the rational method) and a simple flow routing component which both lags in time and attenuates the runoff as it sis transferred to the catchment outlet. The hydrological calculations are based on a water balance equation. The soil erosion uses a modification of the USLE. Phosphorus is transported both as soluble and particulate, with simple conceptualisations of each process. The processes modelled in EPIC are soluble loss in surface runoff, transport by sediments, mineralisation, immobilisation, mineral cycling and crop uptake. Nitrogen is also modelled and EPIC accounts for Nitrate loss in surface runoff, organic-N transport with sediment, dinitrification, mineralisation, immobilisation, crop uptake, fixation and contributions from rainfall.

Data Requirement:
The model requires input from GRASS GIS layers. These include soil series and weather data, although the model can generate the necessary weather parameters. The model also requires management information that can be input from a text file.

Output:
The model provides output on crop yields, economics of fertilizer use and crop values.

Version and System Requirements:
EPIC requires an IMB AT PC or compatible system that has at least 640K of memory and 4 megabytes of disk storage space. The use of a maths coprocessor (8087) is not required, but is recommended.

Application History:
The model was successfully tested at a large number of sites in the US with a wide range of climatic conditions, soil types and management practices.

Availability:
The programme can be downloaded at:

http://www.brc.tamus.edu/epic/downloads/index.html

Website:

http://www.brc.tamus.edu/epic/

ERSEM — European Regional Seas Ecosystem Model

Description:
ERSEM is a comprehensive ecosystem model which dynamically simulates the large scale cycling or organic carbon, oxygen and the macro nutrients N, P and Si over the seasonal cycle in the North Sea. The model consists of an interlinked set of modules, describing the biological and chemical processes in the stratified or non-stratified water column and in the benthic system, as forced by light and temperature. Physical transport is included by driving the model with the output of physical circulation and dispersion models

Data Requirement:
Initial and boundary nutrient concentrations, solar radiation, hydrodynamic driving, river loading. The biology in all setups is exactly the same, with the physical model (usually a hydrodynamical model) providing the spatially and temporally different abiotic information (transport/mixing) to the biology and the biology modifying the abiotic environment (production/consumption).

Output:
Concentrations of each state variable.

Version and System Requirements:
The ERSEM-II project has the objective to test and improve our understanding of the long-term, large-scale dynamic functioning of regional seas and their coastal margins. ERSEM-II is the natural follow-up of the ERSEM-I.

Assumptions and Limitations:
The major problem with ERSEM is the coupling of the biological model to different 3D hydrodynamical models to be used. This coupling preferably is bi-directional, in order to allow the expression of the biology modifying the physical state of the system (e.g. modification of the heatflux into the water column, modifying vertical mixing rates). The biological resolution of the model is high, much too high in the eyes of many non-biologists, much too low in the eyes of many biologists.

Application History:
The model has been applied to aquatic systems ranging from mesocosms in Danish waters Norwegian fjords, and the Northern Adriatic to pseudo- or full 3D setups of the North Sea and the Adriatic. The biology being formulated identically everywhere, but expressing itself widely differently in the different systems it has been applied to, implies that ERSEM is well on its way to meeting its prime objective of being a generic formulation of marine ecosystem function. It has the capability of addressing (and maybe even laying to rest) some of the apparent paradoxes in marine ecology such as bottom-up vs. top-down control, bacterioplankton being a sink or a link to higher trophic levels, the consequences of nutrification at a system level etc.

Availability:
It has been developed, refined and applied in Marine Science and Technology (MAST) projects by shifting consortia of leading marine science institutes in Europe. The model was developed during the European MAST project ERSEM I 1990 - 1993. Structural refinement and several applications were realized in the project ERSEM II 1993 - 1996.

Website:
http://www.nioz.nl/en/deps/bio/projects/ERSEM/Description.html

EUROHARP	European Harmonised Procedures for Quantification of Nutrient Losses from Diffuse Sources

Description:

EUROHARP includes nine different contemporary methodologies for quantifying diffuse losses of N and P, and a total of 17 study catchments across gradients in European climate, soils, topography, hydrology and land use. These methodologies have been selected to include those approaches - applicable at catchment scale - that are currently used by European research institutes to inform policy makers at national and international levels. The first primary objective of EUROHARP is to provide end-users (national and international European environmental policy-makers) with a thorough scientific evaluation of the nine contemporary quantification tools and their ability to estimate diffuse nutrient (N, P) losses to surface freshwater systems and coastal waters. Thereby facilitate the implementation of the EC WFD. The second primary objective is to develop an electronic decision support system (tool-box) for the identification of benchmarking methodologies with respect to both costs and benefits, for the quantification of diffuse nutrient losses under different environmental conditions across Europe. EUROHARP will contribute substantially to improved comparability, transparency and reliability of the quantification of nutrient losses from diffuse sources, and thereby to improved efficiency of abatement strategies related to the implementation of e.g. the Nitrates Directive and the WFD.

Used Models:

EUROHARP includes the following nine different contemporary methodologies for quantifying diffuse losses of N and P: ANIMO; REALTA; N-LES; MONERIS; TRK; SWAT; EVENFLOW; Nopolu and Source Apportionment.

http://www.euroharp.org/

EUTROMOD Evaluation of the Water Quality Model

Description:

The EUTROMOD computer model was developed to provide guidance and information for managing eutrophication in lakes and reservoirs. It is a collection of spreadsheet-based nutrient loading and lake response models which may be used to relate water quality goals to allowable nutrient inputs. The model, thereby, provides information concerning the appropriate mix of point source discharges, land use, and land management controls that result in acceptable water quality. EUTROMOD and appropriate documentation are available from the North American Lake Management Society (NALMS). The model was developed by Ken Reckhow of Duke University as a simple, spreadsheet-based collection of models with built-in uncertainty analysis.

Data Requirement:

The simplicity of EUTROMOD reflects the belief that simple models with thorough uncertainty analysis are valuable tools for watershed and lake management. Therefore, data requirements are moderate. Many input parameters are from well known relationships (e.g. USLE and Rational Formula) and from common soil, topographical, and land management characteristics. The manual consists of many tables and figures to assist in the selection of input parameters. However, it is important that regional or site specific information be used when available. The input parameters alternate between English and SI units. A sample data set is included in EUTROMOD, however, we caution against blind use of these parameter values for specific studies. The most difficult data requirement is the lumping of various soil and topographic parameters by land use. A geographic information system (GIS) can be very useful by allowing one to overlay soil and topographic data layers with land use to obtain mean or area-weighted parameter values.

Output:
The results of EUTROMOD are ultimately designed to predict the trophic state of the lake. Output from the model includes lake nutrient (nitrogen and phosphorus) levels (mg/l), chlorophyll a (ug/l), and Secchi Disk depth (m). In addition, Carlson's TSI is estimated. EUTROMOD also outputs predictions of the average annual runoff volume (106 m3/yr), sediment loading (Mg/yr), dissolved nitrogen and phosphorus (kg/yr), sediment attached nitrogen and phosphorus (kg/yr), and total nitrogen and phosphorus (kg/yr), as produced annually by the contributing watershed. Various pie charts and bar charts are produced automatically to allow for visual comparison of nutrient and sediment loadings attributed to various sources in the watershed. An estimate of uncertainty in the outputs is provided in terms of model error and hydrologic variability. The model error is provided in terms of lake response estimates plus or minus one standard deviation, which is associated with the error term of the regression models. Year-to-year variability is addressed by utilizing a mean precipitation and coefficient of variation to account for hydrologic variability in the output. The hydrologic variability is propagated by utilizing first-order error analysis.

Version and System Requirements:
The original Version 3.0 was converted from As Easy As to Microsoft Excel (Microsoft Corporation, Cambridge, MA). This version has recently been updated to reflect the changes made in Version 3.65 of the As Easy As version described above. In addition, a modification of the Microsoft Excel version that allows for simulating up to 10 sub-watersheds contributing to a lake is in development.

Assumptions and Limitations:
Annual runoff, erosion, and nutrient (nitrogen and phosphorus) loadings are simulated with a simple, lumped watershed modelling procedure. Lake response is predicted by a set of non-linear regression equations from multi-lake regional data sets in terms of lake nutrient levels, chlorophyll *a*, Secchi Disk depth, and a trophic state.

EUTROMOD is intended for predicting lake-wide average conditions for the growing season as a function of annual nutrient loadings. Therefore, short-term conditions (e.g., weekly or monthly), spatially-local water quality (e.g. concentrations in embayments), and dynamic response (e.g. continuous changes over time) cannot be predicted.

Application History:

Extensive evaluation of EUTROMOD has not been performed. However, the model has been used in many different regional areas with success. A study of Wister Lake in Oklahoma found that EUTROMOD results compared well with water quality monitoring data. In addition, the Oklahoma Water Resource Board (OWRB) evaluated EUTROMOD results on the same lake and compared it with several additional models and estimates. They found the EUTROMOD results to be consistent with the other estimation procedures.

Availability:

The spreadsheet program, and a users manual, may be ordered from the North American Lake Management Society, NALMS, at 608-233-2836 or at the NALMS homepage. Cost Software 3.5 in. disk - IBM - (EUTROMOD V3)

Watershed and lake modelling procedure for eutrophication management with an emphasis on uncertainty analysis.

Manual 147 pp.

Item No.: S5

Price: Currently $64 Members / $80 Non-Members + shipping & handling

Website:

http://www.nalms.org/bkstore/software.htm

EVHA	Logiciel d'<u>EV</u>aluation de l'<u>HA</u>bitat

Description:
The user's guide and description of the methodology are available as pdf files in French at the website.

Availability and Website:
The model can be obtained at:

http://www.lyon.cemagref.fr/bea/lhq/software.html

FLOWPATH II

Description:
Flowpath is commercially available from Waterloo Hydrogeological. It is a two dimensional areal, finite difference, groundwater flow, pathline (particle tracking) and contaminant modelling package. It allows the simulation of leaky, confined and unconfined aquifers of anisotropic and heterogenous porous media. It can simulate flow to and from wells, supports recharge, constant head and prescribed flow boundary conditions, including rivers/lakes and drains. Solute transport is simulated with two-dimensional dispersivity, diffusion, first order biological-radioactive decay, and retardation. Only steady state conditions are simulated and there is no probabilistic modelling capability.

Data Requirement:
See 3.3.8 V b) *Data Requirements for distributed flow models*

Output:
Contoured/grid results of hydraulic heads, drawdown, flow velocities, pathlines, calibration residuals, water budget and pollutant concentrations

Version and System Requirements:
Flowpath II is the most recent version of Flowpath (Franz and Guiguer, 1990) developed at Waterloo Hydrogeologic, System Requirements: PC Pentium 100MHz, 32 Mb RAM, SVGA Monitor. O.S.: Windows 98, NT, 2000, XP

Assumptions and Limitations:
See 3.3.8 V b) Number of Dimensions to be modelled in distributed models for discussion

Application History:
Extensively used world wide in industry and research

Availability and Website:
Available to order on-line from Waterloo Hydrogeologic Inc. at http://www.flowpath.com/software/software_main.htm

FLUX Simplified Procedures for Eutrophication Assessment and Prediction

Description:
The FLUX Program allows estimation of tributary mass discharges (loadings) from sample concentration data and continuous (e.g., daily) flow records. Five estimation methods are available and potential errors in estimates are quantified.

Flux can be interrelated with the programmes PROFILE and BATHTUB to simplify assessments of eutrophication-related processes and effects.

Data Requirement:
Requires grab sample concentration data and continuous (e.g. daily) flow records.

Output:
FLUX delivers graphic and tabular displays that allow users to evaluate input data and calculation results. Mass loads, and associated error statistics (CV) are provided as input to BATHTUB.

Version and System Requirements:
MS DOS; PC Compatible.

Availability:

Distributor: Dr. Robert H. Kennedy

Environmental Laboratory

U.S. Army Engineer Waterways Experiment Station

3909 Halls Ferry Road

Vicksburg, MS 39180

kennedr@wes.army.mil

The model can be downloaded at:

http://www.wes.army.mil/el/elmodels/index.html

Website:

http://www.wes.army.mil/el/elmodels/emiinfo.html

GBMBS	***Green Bay Mass Balance Study***

Description:

The Green Bay Mass Balance Study (GBMBS) was conducted in 1989-90 to pilot the technique of mass balance analysis in understanding the sources and effects of toxic pollutants in the Great Lakes food chain. The overall goal of study was to test the mass balance approach for tracking toxicants (mainly PCBs at the congeners level) in a system under additional pressure from nutrients. The integrated modelling framework consisted of a suite of individual models to simulate hydraulics, sorbent dynamics and toxic chemicals in Green Bay, Lake Michigan (Koelmans *et al*., 2001)

The study, headed by EPA's Great Lakes National Program Office (GLNPO) and the Wisconsin Department of Natural Resources, had many participants from the Federal, state, interagency, and academic communities. The study focused on four representative chemicals or chemical classes: PCBs, dieldrin, cadmium, and lead (USEPA, 1989).

Input and Output Data:

The eutrophication model component generates organic carbon-related solids which are input to a long term solid model (GBTS) and a sorbent dynamics model (Green Bay Organic Carbon Sorbent; GBOCS). The output of GBOCS forms an input to the contaminant exposure model (GBTOX) the output of which forms the input to the food chain model.

Assumptions and Limitations:

The PCB model framework included interactions between: air water; water sediment and the food chain.

Application History:

Results of the sub-model component GBTOX were successfully compared with particulate phase and dissolved PCB concentrations that were collected for the GBMB study.

The GBMBS modelling framework was successfully applied to a major follow up project: the Lake Michigan Mass Balance Study (LMMBS) in the Great Lakes.

Availability:

Contact: Dave DeVault

Telephone: 612-296-7253

Email: dave.devault@pca.state.mn.us

Information Type: Data, Text

The GBMBS data sets are available at:http://www.epa.gov/grtlakes/gbdata/gbay2.html

Website:
http://www.epa.gov/grtlakes/gbdata/

Groundwater Vistas

Description:
Groundwater Vistas is a modelling environment and integrated suite of models for 3-D distributed flow and transport modelling using the MODFLOW suite of codes

Version and System Requirements:

Version 3.0 is the most recent version. PC Pentium, at least 64 Mb RAM and 40 Mb of hard-disk space. O.S.: Windows Versions 95, 98, 2000 and NT

Supported Models:
Includes (comes with) MODFLOW, MODPATH and MT3D and supports, that is will run from within the environment, MODFLOW2000, MT3D'99, GFLOW - 2D, MODPATH, PATH3D, MODFLOWT, and MODFLOW-SURFACT and the PEST & UCODE model-independent calibration softwares. Imports data from SURFER & ASCII files and files from MODFLOW, ModelCad & Flowpath. Imports from and exports to the ArcView GIS software. Displays both plan and x-sectional views. Export results to SURFER, Slicer, DXF, BMP, WMF, EarthVision, EVS, Tecplot, & ASCII files for manipulation and display. The Advanced Version of Groundwater Vistas includes probabilistic, Monte Carlo versions of MODFLOW, MODPATH and MT3D.

Availability and Website:
Groundwater Vistas is developed by and available to order online from Environmental Simulations Limited at:

http://www.groundwatermodels.com/software/Software.asp

GLUE **Generalised Likelihood Uncertainty Estimation**

Description:

The GLUE methodology, previously used in rainfall-runoff modelling, is applied to the distributed problem of predicting the space and time varying probabilities of inundation of all points on a flood plain. Probability estimates are based on conditioning predictions of Monte Carlo realizations of a distributed quasi-two-dimensional flood routing model using known levels at sites along the reach. The methodology can be applied in the flood forecasting context for which the *N*-step ahead inundation probability estimates can be updated in real time using telemetered information on water levels. It is also shown that it is possible to condition the *N*-step ahead forecasts in real time using the (uncertain) on-line predictions of the downstream water levels at the end of the reach obtained from an adaptive transfer function model calibrated on reach scale inflow and outflow data

Output:

At each time step the predicted output from the retained runs are likelihood weighted and ranked to form a cumulative distribution of the output variable from which chosen quantiles can be selected to represent model uncertainty.

Application History:

The Generalised Likelihood Uncertainty Estimation (GLUE) framework of Beven and Binley (1992) was used to assess the resulting uncertainty in the predictions. The procedure has been described by Romanowicz *et al.* (1994) as "in essence a Bayesian approach to uncertainty estimation for nonlinear hydrological models that recognises explicitly the equivalence, or near equivalence, of different parameter sets in the representation of hydrological processes".

Availability and Website:

Contact:

Prof. Keith Beven,

Department of Environmental Science, Institute of Environmental and Natural Sciences,Email K.Beven@lancaster.ac.uk. The model can be downloaded for free at: http://www.es.lancs.ac.uk/hfdg/glue.html

GWLF — Generalised Watershed Loading Function

Description:
The GWLF model was developed at Cornell University to assess the point and nonpoint loadings of nitrogen and phosphorus from relatively large, agricultural and urban watershed and to evaluate the effectiveness of certain land use management practices. One advantage of this model is that it was written with the express purpose of requiring no calibration, making extensive use of default parameters. The GMLF model includes rainfall/runoff and erosion and sediment generation components, as well as total and dissolved nitrogen and phosphorus loadings.

Data Requirement:
Loading functions provide a useful means for estimating nutrient loads when chemical simulation models are impractical due to funding limitations or data availability. Much of the data for the GWLF model are available through databases maintained by U.S. state and federal agencies such as the National Weather Service, USDA Soil Conservation Service, planning departments, etc. Other key input parameter can be estimated based on literature research which is summarized in the GWLF User's Manual. The GWLF model uses daily rainfall and temperature data to drive water balance calculations. To determine runoff, the GWLF uses the Soil Conservation Service's (SCS) curve number equation. Another important parameter is the groundwater recession coefficient. This value controls the rate at which saturated soil discharges to the stream. This value can be calculated from gauged flow records. If this data is not available, the data may be used from a neighbouring watershed.

Output:
This model uses daily time steps and allows analysis of annual and seasonal time series. The model also uses simple transport routing, based on the delivery ratio concept. In addition, simulation results can be used to identify and rank pollution sources and evaluate basin wide management programs and land use changes. The model also includes several reporting and graphical representations of simulation output to aid in interpretation of results.

Assumptions and Limitations:
The current versions of this model does not account for loadings of toxins and metal, but with minimal effort improvements can be made to add this feature. For the application of the model to a site in Ireland, where the hydrological conditions are significantly different, the hydrological component of the model must be revisited, checked and validated.

Application History:
The model has been applied to a number of catchments in the USA, such as the Tar-Pimlico basin, the Lake Lanier catchment and the Catskill catchment. The latter is a source for water supply to New York City. It is currently under test for Lough Leane catchment – Killarney (Contact: A. Allott, Centre for Environment, TCD).

Availability:
Contact: Michael McCarthy

Research Triangle Institute

PO Box 12194

Research Triangle Park, NC 27709

Tel: (919) 541-6895

Email: jmm@rti.org

HarmoniQuA	Harmonising Quality Assurance in model based catchment and river basin management 2002-2005

Description:
HarmoniQuA is a research project supported by the European Commission under the Fifth Framework Programme and contributing to the implementation of the Key Action "Sustainable Management and Quality of Water" within the Energy, Environment and Sustainable Development Programme. HarmoniQuA forms part of the CATCHMOD cluster of projects; supporting the implementation of the WFD. It aims to provide a user friendly guidance and QA framework for use in model based river management. It will prompt users with the appropriate 'next step' in the modelling process and provide an audit trail to check previous decisions. The approach targets management at catchment and river basin scales with the overall goal of improving the quality of modelling and therefore enhancing the confidence of all stakeholders in them. HarmoniQuA attempts to serve several types of users in a series of water management domains, in jobs of varying complexity and application. Users working on a specific job will only be confronted with guidance relevant to them in their present context.

Website:

http://harmoniqua.wau.nl/

HBV-N

Description:

The HBV-N model is a process-based, semi-distributed conceptual model, which has recently been used by national authorities in large-scale estimates of Swedish nitrogen (N) load, retention and source apportionment for the Baltic Sea. When applying the model the river basin may be divided into several coupled sub-basins, for which the calculations are made separately, and this gives the spatial distribution of the model results. The hydrological part (i.e. HBV-96) consists of a routine for accumulation and melt of snow, a routine for accounting of soil moisture, and a routine for lake routing and runoff response. The model includes a number of free parameters, which are calibrated against observed time-series of water runoff and N concentrations. For large-scale catchment applications, the calibration procedure is made step-wise with consideration to several monitoring sites in a region. In the N routine, leakage concentrations are assigned to the water percolating from the unsaturated zone of the soil to the response reservoir of the hydrological HBV model. Different concentrations are applied to water originating from the land use categories forest, urban, arable and other land. The arable land may be further divided into a variety of crops and management practices, for which the N leaching is achieved by using the field-scale model SOIL-N. In addition to the diffuse soil-leaching, N is also added from point-sources, such as rural households, industries, and wastewater treatment plants. Atmospheric deposition is added to lake surfaces, while deposition on land is implicitly included in the soil-leaching. The model simulates residence, transformation and transport of N in groundwater, rivers and lakes. The equations used to account for the N turnover processes are based on empirical relations between physical parameters and concentration dynamics. Inorganic N and organic N are treated separately in the simulations and the calculations are made with a daily time-step.

Data Requirement:

Sub-basin characteristics; size and hydrological coupling. Can be achieved from digitalized sub-basin boundaries (water divides).

Daily precipitation from all available climate stations

Daily air temperature from all available climate stations

Potential evapotranspiration

Land use for each sub-basin (forest or open land, lake surface)

Elevation zones in each sub-basin, e.g., from DEM or maps

Approximate depths of larger lakes

Atmospheric N-deposition on lake surfaces

Point-source N

Observed time-series of N in the river

Observed time-series of runoff in the river.

Versions:

The HBV-NP version of the mass balance model takes both nitrogen and phosphorus into account.

Availability:

For further information, please contact:

Dr. Berit Arheimer,

Swedish Meteorological and Hydrological Institute,

SE-601 76 Norrköping,

Sweden.

Email: Berit.Arheimer@smhi.se

Website:

http://www.smhi.se/sgn0106/if/hydrologi/quality.htm

HEC	**<u>H</u>ydrologic <u>E</u>ngineering <u>C</u>enter**

Description:

The Hydrologic Engineering Center (HEC), an organization within the Institute for Water Resources, is the designated Center of Expertise for the US Army Corps of Engineers in the technical areas of surface and groundwater hydrology, river hydraulics and sediment transport, hydrologic statistics and risk analysis, reservoir system analysis, planning analysis, real-time water control management and a number of other closely associated technical subjects. HEC supports Corps field offices, headquarters, and laboratories by providing technical methods and guidance, water resources models and associated utilities, training and workshops, accomplishing research and development, and performing technical assistance and special projects. The products that are developed from these activities are for the Corps but are available to the public and may be freely downloaded from this web site.

Latest Model releases of HEC are:

- HEC – DSSVue 1.0; HEC- RAS 3.1.1; HEC- GeoRas 3.1.1 and HEC- HMS 2.2.2.

Availability:

HEC Fax:

(530) 756-8250

Mailing Address: ‘

Department of The Army
Corps of Engineers
Institute for Water Resources
Hydrologic Engineering Center
609 Second Street
Davis, CA 95616-4687

Webmaster E-mail Address:

hec.webmaster@usace.army.mil

Distributor:

Dr. Robert H. Kennedy
Environmental Laboratory
U.S. Army Engineer Waterways Experiment Station
3909 Halls Ferry Road
Vicksburg, MS 39180
Email: kennedr@wes.army.mil

Website:

http://www.hec.usace.army.mil/default.html

HOC BIOACCUMULATION **Model for shallow aquatic systems**

Description:

"HOC bioaccumulation" is a dynamic environmental fate and population-based food chain accumulation model to determine the influence of varying trophic status on hydrophobic organic compound (HOC) transfer and fate in shallow aquatic systems. The model is based on detailed carbon-based benthic-pelagic food chain and tracks the transfer and accumulation of organic carbon and HOCs among 16 biotic and abiotic pools over time scales from days to years. The following mechanisms of contaminant transfer are included: binding to DOC; the bacterial loop; redistribution through bioturbation and re-suspension events.

Assumptions and Limitations:

The model assumes a spatially homogenous system. Temperature, light and nutrient load are the three forcing functions that drive the production of algal biomass in the modelled system. The three functions are defined over an annual scale. The biomass supports production in the water column and sediment. The food web consists of five trophic levels in the water column: bacteria; protozoa; phytoplankton; zooplankton and piscivores. Three levels are described in the benthic environment: deposit feeder; filter feeder and benthicvores/forage feeders. Both water column and sediment associated POC and DOC pools are incorporated. The carbon exchange at the sediment-water interface is defined by: pelagic species supplying deposit feeders with settling organic matter (e.g. through excretion); filter feeder ingestion of algal and settling POC and carbon recycling to the water column by piscivores grazing on benthic (forage) fish. HOC transfer is described through: diffusion, air-water exchange, bioconcentration, utilisation of DOC or POC; trophic transfer; mortality and excretion losses; sedimentation and re-suspension by bioturbation.

HOC concentrations are assumed to be remain below deleterious levels so that the carbon flows are not altered by toxicity. Therefore, the influence of toxicity is not included in the model.

Application History:
The biomass output of the model was verified and validated with respects to measured periodicity and ranges of values, using data from Chesapeake Bay and the Baltic Sea. However, validation with respect to HOC fate was not yet been done. The model was used to calculate HOC scenarios in aquatic systems with different trophic states.

HSCTM2D Hydrodynamic, Sediment and Contaminant Transport Model

Description:
A finite element modelling system for simulating two-dimensional, vertically-integrated, surface water flow (typically riverine or estuarine hydrodynamics), sediment transport, and contaminant transport. The modelling system consists of two modules, one for hydrodynamic modelling (HYDRO2D) and the other for sediment and contaminant transport modelling (CS2D). HSCTM2D can be run in an uncoupled or semi-coupled mode. In the uncoupled mode, HYDRO2D is run separately from CS2D. In the semi-coupled mode, HYDRO2D and CS2D are run in the following fashion. First, HYDRO2D calculates the flow field for the current time step. Second, the predicted flow field is used in CS2D to calculate the transport of sediments and contaminants during the same time step. HYDRO2D is run at every time step to update the flow field to account for predicted changes in nodal flow depths due to erosion and deposition. HYDRO2D solves the equations of motion and continuity for nodal depth-averaged horizontal velocity components and flow depths. The effects of bottom, internal and surface shear stresses, horizontal salinity gradients, and the Coriolis force are represented in the equations of motion. CS2D solves the advection-dispersion equation for nodal vertically-integrated concentrations of suspended sediment, dissolved and sorbed contaminants, and bed surface elevations. The processes of dispersion, aggregation, erosion, deposition, adsorption and desorption are simulated. A layered bed model is used in simulating bed formation and subsequent erosion.

Output:
Sediment bed structure (density and shear strength profiles, thickness and elevation), net change in bed elevation and net vertical mass flux of sediment over time, average amount of time sediment particles are in suspension, and the downward flux of sediment onto the bed may be output along with scour rates and/or sedimentation erosion/deposition rates, contaminant transport and fate.

Version and System Requirements:
Operating System:16-bit MS-DOS.

Assumptions and Limitations:
HSCTM2D has a default option that will allow the user to make relative comparisons between sites or designs with limited data. To obtain a quantitative analysis, the user must run the non-default option with a complete set of data.

Availability and Website:
Contact:

Center for Exposure Assessment Modelling (CEAM)

National Exposure Research Laboratory - Ecosystems Research Division

Office of Research and Development (ORD)

U.S. Environmental Protection Agency (U.S. EPA)

960 College Station Road

Athens, Georgia 30605-2700

The model can be downloaded for free at:

http://www.epa.gov/ceampubl/swater/hsctm2d/

HSPF Hydrological Simulation Program—Fortran

Description:

HSPF simulates for extended periods of time the hydrologic, and associated water quality, processes on pervious and impervious land surfaces and in streams and well-mixed impoundments. HSPF uses continuous rainfall and other meteorological records to compute streamflow hydrographs and pollutographs. HSPF simulates interception soil moisture, surface runoff, interflow, base flow, snowpack depth and water content, snowmelt, evapotranspiration, ground-water recharge, dissolved oxygen, biochemical oxygen demand (BOD), temperature, pesticides, conservatives, faecal coliforms, sediment detachment and transport, sediment routing by particle size, channel routing, reservoir routing, constituent routing, pH, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, organic phosphorus, phytoplankton, and zooplankton. Program can simulate one or many pervious or impervious unit areas discharging to one or many river reaches or reservoirs. Frequency-duration analysis can be done for any time series. Any time step from 1 minute to 1 day that divides equally into 1 day can be used. Any period from a few minutes to hundreds of years may be simulated. HSPF is generally used to assess the effects of land-use change, reservoir operations, point or non-point source treatment alternatives, flow diversions, etc. Programs, available separately, support data pre-processing and post-processing for statistical and graphical analysis of data saved to the Watershed Data Management (WDM) file.

Data Requirement:

Meteorological records of precipitation and estimates of potential evapotranspiration are required for watershed simulation. Air temperature, dewpoint temperature, wind, and solar radiation are required for snowmelt. Air temperature, wind, solar radiation, humidity, cloud cover, tillage practices, point sources, and (or) pesticide applications may be required for water-quality simulation. Physical measurements and related parameters are required to describe the land area, channels, and reservoirs.

Output:

Output is either printed tables at any time step, a flat file, or the WDM file. The post-processing software uses data from the WDM file. Hundreds of computed time series may be selected for the output files.

Version and System Requirements:
HSPF is written in Fortran 77 with the following extension: use of include files. The HSPF, HSPNODSS, WDM, ADWDM, and UTIL libraries from LIB are required to recompile.

Assumptions and Limitations:
HSPF assumes that the "Stanford Watershed Model" hydrologic model is appropriate for the area being modelled. Further, the instream model assumes the receiving water body model is well-mixed with width and depth and is thus limited to well-mixed rivers and reservoirs. Application of this methodology generally requires a team effort because of its comprehensive nature.

Application History:
The model was developed in the early 1960's as the Stanford Watershed Model. In the 1970s, water-quality processes were added. Development of a Fortran version incorporating several related models using software engineering design and development concepts was funded by the Athens, Ga., Research Lab of EPA in the late 1970s. In the 1980s, pre-processing and post-processing software, algorithm enhancements, and use of the USGS WDM system were developed jointly by the USGS and EPA. The current release is Version 11. An interactive version was developed by the USGS in the 1990s.

Availability:
Operation and Distribution:

U.S. Geological Survey

Hydrologic Analysis Software Support Program

437 National Center

Reston, VA 20192

h2osoft@usgs.gov

Official versions of U.S. Geological Survey water-resources analysis software are available for electronic retrieval at:

http://water.usgs.gov/software/and via anonymous File Transfer Protocol (FTP)

Website:

http://water.usgs.gov/software/hspf.html

HYDROTEL

Description:
Six hydrological processes are simulated by the HYDROTEL model:

* Interpolation of meteorological data
* Accumulation and melt of snow cover
* Potential evapotranspiration
* Vertical water budget
* Surface and sub-surface runoff
* River routing

For specific processes, HYDROTEL offers the possibility of choosing among various sub-models depending on available meteorological data. Thus, when the necessary data are available, it is possible to choose more accurate sub-models based on physical processes. Otherwise, more conceptual sub-models compatible with the available data may have to be chosen. This allows application of HYDROTEL to a very large number of basins, using the best available data (Fortin *et al*., 1995).

History:
The HYDROTEL model has been applied to watersheds located in Québec, Ontario and British-Colombia in Canada and to one in Southern France, in order to test its applicability to watersheds of different types and areas in various climates.

Availability:
Jean-Pierre Fortin, INRS-Eau, Université du Québec, CP 7500, Ste-Foy (Québec), G1V 4C7 CANADA

Fax: + (418) 654-2600

Internet: jp_fortin@inrs-eau.uquebec.ca

Website:

http://www.hydrotel2000.com/

IHACRES **Identification of unit Hydrographs And Component flows from Rainfall, Evaporation and Streamflow data**

Description:
Developed jointly by the Centre for Ecology and Hydrology, Wallingford, UK and the Centre for Resource and Environmental Studies at the Australian National University, Canberra, IHACRES simulates streamflow using only time series data of rainfall, streamflow and temperature without catchment descriptive data. Unit hydrographs for total streamflow and, in many cases, dominant quick and slow flow components can be identified. The model has two modules: non-linear conversion of rainfall to effective rainfall; linear conversion of effective rainfall to streamflow (using a linear, conceptual, unit hydrograph model). The hydrograph module is flexible so that the operator can choose to run the model with a single storage, two storages in series or parallel etc. The number of model parameters depends on the users choice of number of storages, but a model with two storages in parallel has 6 parameters.

Data Requirement:
Observed rainfall and streamflow at regular time intervals; and index data for evaporation, e.g. air temperature, or pan evaporation measurements.

Output:
A range of operator-selected graphical displays and output files of the main results and observed and modelled time series. A summary file appears on the screen automatically after each run (calibration or simulation).

Version and System Requirements:
In the PC-IHACRES version of the model, the parameter optimisation methodology uses an instrumental variable technique to identify the unit hydrograph parameters.

Application History:

The IHACRES methodology has been successfully applied to catchments with catchment areas ranging from 90 m^2 (with 6-minute time steps) to nearly 10,000 km^2 (with monthly data). Applications include characterizing the quick and slow flow dynamics of hydrological regimes; hydrograph separation; and assessing the impacts of land-use change.

Availability:

The software can be obtained from:

Centre of Ecology and Hydrology
CEH Directorate
Internet Communications Officer
Abbots Ripton
HUNTINGDON
Cambridgeshire
PE28 2LS
http://www.ceh.ac.uk/products_services/software/
For further information on IHACRES. Email Dr Ian Littlewood: igl@ceh.ac.uk

Website:

http://dataserv.cetp.ipsl.fr/AIMWATER/hydromodels/IHACRES.html

IFEM	***I**ntegrated **F**ates and **E**ffects **M**odel*

Description:
IFEM is a combination of the toxic effect model SWACOM and the dynamic fate model FOAM. The model is designed for PAHs and accounts for sorption to suspended and settled solids, dissolved organic matter (DOM), detritus and sediment, volatilisation, photolysis and uptake and depuration by the model populations.

The foodweb consists of 11 functional groups. The biomass is calculated from daily light conditions, temperature and predator-prey relationships. Sublethal effects on growth processes are determined using dose-effect and time-varying body burdens, calculated from uptake, degradation and depuration. The effect is modelled using a population specific toxic effect factor, adjusting the rate of population growth (Bartell *et al*., 1988 and Bartell *et al*., 1992).

Assumptions and Limitations:
Nutrients are not included in model.

Application History:
IFEM has been used to study the fate and effects of naphthalene in the water column and shore of a freshwater lake in a temperate climate zone, but has so far not been validated.

INCA	INtegrated CAtchment Model

Description:
Model of hydrology, N, P Sediments , Macrophytes, epiphytes and phytoplankton for application to small and large catchments. Daily time step, dynamic and process model which can be used to investigate impacts of nutrient change, land use change and climate change

Data Requirement:
Daily rainfall, soil moisture deficit, temperature and solar radiation, observed instream data at whatever frequency is available.

Output:
Daily simulations of all variables at each reach boundary along a river system plus annual flux information, profiles down river and 3D plots.

Version and System Requirements:
Runs on PC- windows application

Assumptions and Limitations:
Knowledge of initial soil conditions, cannot differentiate between algal species

Application History:
Applied to 10 UK catchments and 8 EU catchments from Finland to Spain

Availability:
INCA-N is available from p.g.whitehead@reading.ac.uk

INCA-P is still in testing mode

Website:

http://www.reading.ac.uk/INCA

LOICZ

Description:

The LOICZ project commenced in 1993 with the establishment of the International Project Office (IPO) at the Netherlands Institute for Sea Research (NIOZ), Texel - The Netherlands. The Office is financially supported by the Dutch Government and, like all IGBP projects, LOICZ is scheduled to run for 10 years. LOICZ is now in its second 5-year phase. In comparison with the relatively uniform environment of the sunlight zone of the open ocean, or the rapidly mixed environment of the atmosphere, the spatial and temporal heterogeneity of the world's coastal zones is considerable. There are as a consequence considerable methodological problems associated with developing global perspectives of the role of this compartment in the functioning of the total Earth system. Identifying and quantifying this role and developing scenarios of change in the coastal compartment of the Earth system under anthropogenic and geocentric driving forces of change will require a considerable body of research. The LOICZ Implementation Plan provides a blueprint of research and integrative activities ideal to fully meet the project goals. Research and Tasks described in each Focus, provide a design of individual and national research contributing to the overall goals of LOICZ. Framework activities provide mechanisms for coordination and consolidation of the research results. Unlike many of the other Core Projects of the IGBP, LOICZ deals with a specific domain rather than a process and that domain is spatially extremely heterogeneous. To achieve the overall goals and objectives a truly global network of coastal scientists must be developed and the active participation of scientists from developing countries is vital to the ultimate success of this project. Some funding and other support is provided through the Core Project to foster the research envisaged as being undertaken in such countries since their coastlines encompass the bulk of the world's tropical shores and are areas where the rates of anthropogenically driven change are considerable. Whilst the objective of LOICZ is not to undertake coastal zone management a clearly goal is to provide a sound scientific basis for the future sustainable use and integrated management of these environments, under conditions of global change.

Website: http://www.nioz.nl/loicz/

MAGPIE	**Modelling AGricultural Pollution and Interactions with the Environment**

Description:

The MAGPIE Decision Support System (DSS) was developed by the Environment Modelling and GIS Group at ADAS Wolverhampton. The system integrates nitrate leaching models with a national environment database, including information on long-term mean climate (obtained from the Meteorological Office) and soil attributes (obtained from the Soil Survey and Land Research Centre). Available land use data includes the MAFF Agricultural Census, comprising areas of crops and numbers of livestock recorded at the parish scale. The spatial precision of the census land use data has been significantly improved through integration with the Institute of Terrestrial Ecology's (ITE) Land Cover Map of Great Britain, derived from satellite imagery. The DSS enables the user to select areas of interest within England and Wales, for which a project file is created. Project areas analyse in detail a selection of co-operative agreements, by exploring their history, economic and ecological efficiency; investigate the role of co-operative agreements in realising more rational water use; identify special measures needed to establish co-operative agreements in the EU on a larger scale; compare the economic efficiency and ecological effectiveness of co-operative agreements with that of economic instruments and regulations. Based on the research, recommendations will be put forward about the potential use of co-operative agreements in future EU water policy and in reforming the Common Agricultural Policy (CAP). The project is being undertaken by INFO in Germany, DLO-LEI in the Netherlands and WRc in the UK (Lord and Anthony, 2000).

MIKE 11 Hydrodynamic Model

Description:
Mike 11, developed by the Danish Hydraulic Institute / water Quality Institute is similar to the model ISIS in that it is one dimensional fully hydrodynamic software package which can be used to undertake studies in river dynamics and water quality. Like ISIS it is modular with hydrodynamic, rainfall-runoff (hydrological) and quality modules. The water quality module allows BOD and DO modelling and includes *E. coli*, but does not include the full oxygen or nitrogen cycles.

Output:
Output from the hydrodynamic module can be routed to additional modules that simulate the transport of cohesive and non-cohesive sediment, dissolved oxygen, nutrients, heavy metals, and eutrophication.

Version and System Requirements:
MIKE11 is available for Windows 95/98 and Windows NT platforms. Hardware requirements for MIKE 11 are therefore similar to requirements for utilizing Windows platforms. The recommended minimum configuration is:
Pentium processor, 200 MHz
64 MB memory (RAM)
1 GB hard drive
SVGA monitor, resolution 1024x768
1 MB memory on graphics card
*8 x speed CD-ROM drive

Assumptions and Limitations:
Limitations of the software are that the quality processes are not fully comprehensive and that the computational methodology has not been updated and is less stable in some areas than other similar software. Simulation of hydraulic structures is limited.

Availability:

Developer: Danish Hydraulic Institute (DHI)

Contact: DHI Software Support Center

Phone: +45 45 179 333

Fax: +45 45 179 200

email: software@dhi.dk

MIKE11 version 2002 D and 1999 B can be downloaded at:

http://www.dhisoftware.com/mike11/Download/

Website:

http://www.dhisoftware.com/mike11/

MIKE 21 Hydrodynamic Model

Description:
A modelling system for 2D free-surface flows that can be applied in lakes, estuaries, bays, coastal areas, and seas where stratification can be neglected. Water quality modules simulate the fate and transport of conservative or linearly decaying constituents, eutrophication processes including nutrient cycling, phytoplankton, zooplankton, and benthic vegetation growth, processes affecting dissolved oxygen, exchange of metals between the bed sediments and the water column, and sediment transport/deposition/erosion.

Data Requirement:
Boundary hydrodynamics, riverine / marine fluxes, parameter-specific characteristics.

Output:
MIKE 21 is provided with a graphical user interface (Windows 95/98/NT) and a pre- and post-processing module for use in data preparation, analysis of simulation results and graphical presentation including the parameters:

- temperature
- salinity
- coliform bacteria
- nitrogen
- biochemical oxygen demand
- algae
- phosphorus
- dissolved oxygen
- user-defined constituent
- zooplankton
- detritus
- cohesive sediments
- noncohesive sediment
-metals

Version and System Requirements:
MIKE 21 is provided with a graphical user interface (Windows 95/98/NT) and a pre- and post-processing module for use in data preparation, analysis of simulation results and graphical presentation.

Application History:
MIKE 21 has been applied to a wide range of hydraulic phenomena, including tidal currents, storm surges, secondary circulations (eddies and vortices), harbour seiching, dam-breaks, and tsunamis. MIKE 21 also includes modules for wind-wave prediction. MIKE 21 is used widely worldwide.

Application History:

Availability:
Developer: Danish Hydraulic Institute (DHI)

Contact: DHI Software Support Center

Phone: +45 45 179 333

Fax: +45 45 179 200

email: software@dhi.dk

MIKE 21 can be downloaded at:

http://www.dhisoftware.com/mike21/Download/

Website:

http://www.dhisoftware.com/mike21/

MLF	MICRO LOW FLOWS

Description:
The Low Flows 2000 software system consists of a map-based user interface, an underlying universal data base and a low flow estimation module. The system enables natural flow estimates to be derived for any river reach in the United Kingdom and enables the impact of artificial influences on the flow regime to be modelled.

Data Requirement:
At the core of Low Flows 2000 is the CEH Universal feature database model. Complicated data structures can be readily defined within the database model and data may be displayed and manipulated via the graphical user interface. Point data with complex relational structure, such as abstraction licences, and time series data, such as flow records are easily stored and manipulated.

Output:
Annual and monthly natural flow duration curves are predicted for ungauged catchments based on the flow regimes of catchments identified as being hydrogeological similar to the un-gauged, target catchment. Flow frequency curves and monthly mean flows may also be predicted

Version and System Requirements:
The user interface for Low Flows 2000 is a Windows based design using ESRI Map Objects. The Geographic Information System (GIS) based data visualisation enables the User to import and display a variety of different spatial data set

Availability:
Contact:
Software Sales and Support, Institute of Hydrology, Wallingford, Oxfordshire, OX10 8BB, United Kingdom. Tel: +44 (0) 1491 838800; Facsimile +44 (0) 1491 692424 Telex:849365 HYDROL G; E-Mail: Directly Mail to softdev@ioh.ac.uk

Website:

http://www.nwl.ac.uk/ih/www/products/iproducts.html

MODFLOW

Description:
MODFLOW is a 3-D finite difference code which has a modular structure that allows it to be easily modified to adapt the code for a particular application. It simulates steady and transient flow in an irregularly shaped flow system in which aquifer layers can be confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can be simulated. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotropic (restricted to having the principal directions aligned with the grid axes), and the storage coefficient may be heterogeneous. Specified head and specified flux boundaries can be simulated as can a head dependent flux across the model's outer boundary. A parameter estimation programme is built in.

MODFLOWK-GWT is an enhanced version of MODFLOW-2000 from the USGS that incorporates the additional capability to simulate solute-transport processes and compute changes in concentration of a dissolved chemical constituent due to advection, hydrodynamic dispersion, retardation, decay, matrix diffusion, and mixing with multiple fluid sources.

Data Requirement:
See chapter 5, section 5.10, *'Data Requirements for distributed flow models'*

Output:
Contoured/grid results of hydraulic heads, drawdown, flow velocities calibration residuals, local and global water budgets. Post-processors are needed for user – friendly visualisation. MODFLOWK-GWT also: Contaminant concentration distributions, time slices, mass balance results

Version and System Requirements:
The current version of MODFLOW from the USGS is MODFLOW-2000. This and older versions are integrated into current MODFLOW based modelling suites.

System Requirements: PC Pentium, at least 64 Mb RAM and 40 Mb of hard-disk space

O.S.: Windows 95,98 NT, 2000 and workstations

Application History:
MODFLOW has become the industry standard in 3-D modelling software. The USGS has developed associated particle tracking and contaminant transport models, as well as other supporting modelling tools and input and display pre-and post-processors. Other organisations and commercial companies have developed particle tracking and contaminant transport models which take their input flow data from MODFLOW, as well as tools and pre- and post-processors.

Availability:
MODFLOW is developed by and available as freeware to download from the USGS at http://water.usgs.gov/nrp/gwsoftware. It is also included in numerous modelling suites e.g. Groundwater Vistas, Processing MODFLOW and Visual MODFLOW (See 3.3.8 V b) Choice of software and Groundwater Vistas this Annex)

Associated programmes, pre- and post –processors available as freeware from the USGS include:

Model Viewer Vers. 1.0

MFI2k Data input program for MODFLOW-2000

GW_Chart Vers. 1.3.1.0

ZONEBDGT Vers. 2.1, computes sub-regional water budgets for MODFLOW

RADMOD Vers. 1.1, a pre-processor to MODFLOW to simulate axisymmetric problems.

GIS TOOLS for converting MODFLOW output data to GIS data

Website:

http://water.usgs.gov/nrp/gwsoftware

MODPATH

Description:
MODPATH is a particle tracking post-processing package that was developed to compute tree-dimensional flow paths using output from steady-state or transient groundwater flow simulations by MODFLOW. It uses a semi-analytical particle-tracking scheme.

Data Requirement:
Head distribution result from MODFLOW 3-D flow model

Output:
Flow field described by flow paths and flowlines

Version and System Requirements:
System Requirements: PC Pentium, at least 64 Mb RAM and 10 Mb of hard-disk space. O.S.: Windows Versions 95, 98, and NT.

Assumptions and Limitations:
Assumption that particles in a flow system move by advection.

Application History:
Extensively used in industry and research.

Availability and Website:
MODPATH is developed by and available to download as freeware from the US Geological Survey at http://water.usgs.gov/nrp/gwsoftware

MT3D99

Description:
MT3D99 is a three-dimensional numerical model for simulating solute transport in complex hydrogeologic settings, either 2 or 3 dimensional. MT3D is designed to be used in conjunction with any block-centred finite-difference model such as MODFLOW. Like MODFLOW it has a modular structure, making it possible to simulate transport processes independently or jointly, depending on which process(es) dominate. MT3D is capable of modelling advection in complex steady-state and transient flow fields, anisotropic dispersion, first-order decay and production reactions, and linear and non-linear sorption. This version can simulate multi-species reactions and assess natural attenuation within a contaminant plume. Includes a dual porosity model for estimation of mass transfer in fractured media or extremely heterogeneous media. MT3D can be run in probabilistic mode in the Groundwater Vistas Advanced version and Processing MODFLOW Pro modelling suites

Output:
Contour or gridded results of contaminant concentration distributions, time slices, mass balance results for individual or combined processes and single or multi-species reactions. Recommended visualisation of output through a post-processor by e.g. Visual MODFLOW.

Version and System Requirements:
MT3D99 is the most recent version.

System Requirements: Pentium PC, source code also available for implementation on workstation or Macintosh O.S.: Windows 95, NT, 98.

Assumptions and Limitations:
See chapter 5, section 5.10, *'Full (Distributed) Pollutant Transport Modelling'*

Application History:
Extensively used in industry and research.

Availability and Websites:
MT3D99 is developed by S.S. Papadopulos & Associates, Inc. and is available by to order on line from them at http://www.sspa.com/products. Other suppliers include Waterloo Hydrogeologic at http://www.flowpath.com, and Scientific Software Group at http://www.scisoftware.com

N-CYCLE **Nitrogen cycle**

Description:
N CYCLE is a computer-assisted learning (CAL) module. It is a model of the nitrogen cycle which calculates the amounts of nitrogen in the major transformations of the nitrogen cycle in grazed grassland. It presents the results as a dynamic display, with which the user can interact. The calculations relate to a full grazing season. Although designed for grassland grazed by beef cattle the program allows the user to select a dairy system or a 'cutting only' system with no grazing animals. The programme is intended for the use by agricultural students, scientists and advisors. Sub-models in this simulation have been derived partly from extensive studies conducted at IGER over several years and partly from other published information. The programme represents in a novel way the effects of many of the relationships that govern the flow of nitrogen in a farming system. The DOS version of N Cycle is already well-established as a teaching tool. The new Windows version incorporates recent developments in the core model itself as well as simplifying the student's interactions with the model.

Data Requirement:
Site-specific parameters to the model are set and adjusted using graphical controls.

Once site parameters are set, the computer calculates the amount of nitrogen mineralised from the soil organic matter and the consequent fluxes of nitrogen through the various component 'pools' of the nitrogen cycle. The results are displayed on a screen which allows some components of the model to be varied and the immediate recalculation of the model.

Output:
The graphing tool added to the Windows version allows the user to selectively present the response of certain parts of the cycle to changing input parameters e.g. to study the effect on leachates of increasing fertiliser input. Both the graph and the underlying data table can be exported via the Windows clipboard for incorporation into reports.

Availability:
Contacts:
David Lockyer
Institute for Grassland and Environmental Research, North Wyke, Devon

David Scholefield
Institute for Grassland and Environmental Research, North Wyke, Devon

Bryan Dawson
Centre for Computer-based Learning in Land Use and Environmental Sciences (CLUES), University of Aberdeen

Website:

http://www.clues.abdn.ac.uk:8080/mert_idx.html.

NLEAP **Nitrate Leaching and Economic Analysis Package**

Description:
NLEAP is a field-scale computer model developed to provide a rapid and efficient method of determining potential nitrate leaching associated with agricultural practices. It uses basic information concerning on-farm management practices, soils, and climate to project N budgets and nitrate leaching indices. NLEAP calculates potential nitrate leaching below the root zone and to ground water supplies. NLEAP has three levels of analysis to determine leaching potential: an annual screening, a monthly screening, and an event-by-event analysis (Shaffer *et al.,* 1991).

Data Requirement:
Model needs soils, climate, and management data as inputs.

Output:
Tables, graphs, and written text output. Monthly and annual output-drainage volume, NO3, residual N. Temporal Scale: Event based to monthly to annual. Spatial Scale: Field scale to regional (with GIS).

Version and System Requirements:
IBM AT 286, 386, 486, or pentium compatible system, the use of a math coprocessor is recommended. At least 640K of memory; DOS version 2.1 or newer; 4.5 megabytes of disk storage space. NLEAP may be run with either a monochrome or colour monitor; Program execution is unpredictable if any memory resident programs are loaded.

Assumptions and Limitations:
DOS NLEAP is only Windows 95, 98, 2000 compatible through an MSDOS window. Modelling soil nitrogen processes in organic soils is not currently available. Their inclusion will require additional research and modelling efforts. NLEAP does not predict yield reductions caused by pests or nutrient deficiencies. However, the user should consider the effects of these problems when estimating crop yield. The model should not be used where rapid water infiltration, leaching, denitrification, and ammonium volatilisation require time steps smaller than 1 day.

Other situations that should not be modelled include those in which water and solute transport in an aquifer are important considerations, complex layering in the soil profile exists, or a shallow water table supplies crop needs. Sequential year runs involving complex crop rotations are difficult to simulate.

Availability and Reference:

USDA-ARS-NPA, Great Plains Systems Research Unit, P.O. Box "E", Fort Collins, Colorado USA, 80522

Phone Number: (970) 490-8300

Fax Number: (970) 490-8310

Email: GPSR_Email@ars.usda.gov

The software can be freely downloaded at:

http://www.or.nrcs.usda.gov/water/wqtools.htm#nleap

Website:

http://gpsr.ars.usda.gov/products/nleap/nleap.htm

N-LES	Nitrate Leaching EStimator

Description:
N-LES estimates N leaching from the root zone and requires inputs data of: total-N added in spring and autumn; an estimate of N left by grazing animals; N fixation by leguminous plants; timing of ploughing in of grass; soil type; water percolation through root zone; and crop type. A separate model EVACROP, estimates transpiro-evaporation and water percolation.

Data Requirement:
Level of total-nitrogen added in the crop rotation; fertilization in spring; autumn fertilization; nitrogen left by grazing animals; nitrogen fixation by leguminous plants; timing of ploughing-in of grass; soil type; water percolation through the root zone; crop type (main crop and winter or catch crop)

Assumptions and Limitations:
Only valid within the range of the calibration data set. Less dynamic. For use in other agro-climatic regions than Denmark the model needs a calibration data set from experimental fields which for some countries/regions might be lacking. Some factors influencing nitrogen leaching – e.g. the effect of an unsuccessful harvest – are not included in the model.

Availability:

Main contact:

Hans Estrup Andersen
Nat. Env. Research Inst.
Vejlsøvej 25, p.o.box 314
DK-8600 Silkeborg, Denmark
phone +45 89 20 14 00
email hea@dmu.dk

Alternative contact:

Brian Kronvang
Nat. Env. Research Inst.
Vejlsøvej 25, p.o.box 314
DK-8600 Silkeborg, Denmark
phone +45 89 20 14 00
email bkr@dmu.dk

Website:

http://www.euroharp.org/pd/pd/models/Nles-short.htm

NTWRK **Analysis of Ecological Flow Networks**

Description:
Network analysis is a phenomenological approach that holistically quantifies the structure and function of food webs by evaluating biomasses and energy flows. The efficiency with which energy and material is transferred, assimilated, and dissipated conveys significant information about the structure and function of food webs (Baird and Ulanowicz 1989 / 1993; Baird *et al.* 1991; Ulanowicz and Wulff 1991). Network analysis has been used to compare ecosystems of different size, geographical location, hydrological characteristics, and trophic status (Baird *et al.* 1991; Ulanowicz and Wulff 1991; Baird and Ulanowicz 1993; Monaco and Ulanowicz 1997). Most recently, arguments have been advanced for the use of network analysis to quantify the health and integrity of ecosystems (Ulanowicz, 2000) and to evaluate the magnitude of stress imposed on an ecosystem (Ulanowicz, 1995). There are fundamentally four types of analyses in network analysis: (1) input/output analysis, (2) the determination of trophic status and the identification of an equivalent linear food chain, (3) elaboration and analysis of biogeochemical cycling and the supporting flows, and (4) calculation of ecosystem indices (or properties) derived from information theory that describe the state of the food web.

Data Requirement:
All of the routines contained herein require data on the entire network of exchanges of a particular medium (energy or some form of matter). Sometime prior to data collection assumptions had to have been made on how the ecosystem (or other system) was to be aggregated into compartments. For each compartment it is necessary to know: (1) all the inputs from outside the system, (2) all the various inputs flowing from other compartments of the system, (3) all the outputs which flow as inputs to other compartments, (4) all exports of useful medium outside the system, and (5) all rates of dissipation of medium.

Version and System Requirements:
EcoNetwrk is based on the text-based application 'Netwrk 4.2' by Robert E. Ulanowicz. EcoNetwrk performs all of the analysis of Netwrk 4.2 but in a windows friendly environment. Netwrk 4.2 is copyrighted (1982, 1987, 1998, 1999).

Availability:
Contact:

University of Maryland

Center for Environmental &

Estuarine Studies

Chesapeake Biological Laboratory

Solomons, MD 20688-0038

Tel: (410) 326-7266

FAX: (410) 326-7378

mailto:ulan@cbl.umces.edu

Website:

http://www.cbl.cees.edu/~ulan/ntwk/network.html

PAEQANN **Predicting Aquatic Ecosystem Quality using Artificial Neural Networks**

Description:

The goal of the project is to develop general methodologies, based on advanced modelling techniques, for predicting structure and diversity of key aquatic communities (diatoms, micro-invertebrates and fish), under natural (i.e. undisturbed by human activities) and under man-made disturbance (i.e. submitted to various pollutions, discharge regulation). Such an approach to the analysis of aquatic communities will make it possible to:

i) set up robust and sensitive ecosystem evaluation procedures that will work across a large range of running water ecosystems throughout European countries;

ii) predict biocenosis structure in disturbed ecosystems, taking into account all relevant ecological variables;

iii) test for ecosystem sensitivity to disturbance;

iv) explore specific actions to be taken for restoration of ecosystem integrity.

Our investigations will therefore help to define strategies for conservation and restoration, compatible with local and regional development, and supported by a strong scientific background. Among the available modelling techniques, artificial neural networks are particularly appropriate for establishing relationships among variables in the natural processes that shape ecosystems, as these relationships are frequently non-linear. LFE (Laboratory of Freshwater Ecology, URBO, FUNDP) is in charge of coordinating the work on benthic diatom communities.

Website:

http://www.fundp.ac.be/urbo/paeqann.html

PHABSIM	**Physical HAbitat SIMulation**

Description:
This extensive set of programs is designed to predict the micro-habitat (depth, velocities, channel indices) conditions in rivers as a function of streamflow, and the relative suitability of those conditions to aquatic life. PHABSIM models were developed to analyse and display the relationship between streamflow and physical habitat, or between streamflow and recreational river space. This relationship is a function between the physical habitat and the streamflow. It can be used to examine the trade-off between the value of water used instream with the water used out-of-stream. Therefore, tradeoffs can be made between alternative uses and mutually acceptable management criteria developed. The decision as to the "best" allocation of the available water is a matter of negotiation among various interest groups. The Instream Flow Incremental Methodology (IFIM) provides a framework for applying PHABSIM in a water resource decision setting. Download Stream Habitat Analysis Using the Instream Flow Incremental Methodology from the FORT web site for a comprehensive introduction to IFIM.

Data Requirement:
Extensive input of hydrological and habitat conditions.

Output:
Optimisation procedure that predicts suitability for fish (mainly salmonid) survival.

Version and System Requirements:
Windows 95

Application History:
PHABSIM has been used in the USA, France, Norway, New Zealand, Canada and Australia.

Availability:
U.S. Geological Survey, 2150 Centre Avenue, Bldg C, Fort Collins, CO 80526-8118

The phabsim software is available as a free download at

http://www.fort.usgs.gov/products/software/software.asp

Website:

http://www.fort.usgs.gov/products/software/phabsim/phabsim.asp

PHOSMOD

Description:
This dynamic model calculates the effects of soil-phosphate, starter-fertiliser-phosphate and granular fertiliser phosphate on daily crop growth, phosphate concentration in the plant, and the changes in the different forms of soil phosphate. It is mechanistic and largely based on well-known equations for key processes. The inputs are generally easy to obtain.

Availability:

Contact:

D. J. Greenwood

Horticulture Research International, Wellesbourne, UK

Phone:

Fax:

email: duncan.greenwood@hri.ac.uk

Software 3.5 in. disk - IBM - (PHOSMOD V1.0)

Describes a modelling framework that is designed to assess the impact of phosphorus loading on stratified lakes.

Manual 20 pp.

Item No.: S7

Price: Currently: $64 Members / $80 Non-Members + shipping & handling

Website:

http://www.nalms.org/bkstore/software.htm

PLUME-RW	Pollutant dispersion

Description:
PLUME-RW is a well-established model developed for studies of pollutant dispersion in estuaries and coastal waters linked to the TELEMAC model. Typically, PLUME-RW is used to optimise outfall location and waste treatment levels.

Data requirement:
PLUME-RW uses flow data derived using TELEMAC to simulate transport by prevailing currents, turbulent dispersion, bacterial decay and deposition and re-suspension of particulates at the sea bed.

Output:
Both dissolved pollutants, such as bacteria from sewage discharges, and suspended pollutants, such as sediment released during dredging operations, can be simulated.

Availability:
Contact:HR Wallingford Ltd,
Howbery Park, Wallingford,
Oxfordshire, OX10 8BA,
United Kingdom
Tel: +44 (0) 1491 835381
Fax: +44 (0) 1491 832233
mailto:info@hrwallingford.co.uk

Website:
http://www.hrwallingford.co.uk/software/telemac.html - top

PLUMES

Description:
This is a near-field model. PLUMES includes two initial dilution plume models (RSB and UM) and a model interface manager for preparing common input and running the models. Two farfield algorithms are automatically initiated beyond the zone of initial dilution. PLUMES also incorporates the flow classification scheme of the Cornell Mixing Zone Models (CORMIX) with recommendations for model usage, thereby providing a linkage between the systems. PLUMES models are intended for use with plumes discharged to marine and some freshwater bodies. Both buoyant and dense plumes, single sources, and many diffuser outfall configurations can be modelled.

Version and System Requirements:
Current Version: 3.0

Operating System:16-bit MS-DOS

Availability and Website:
U.S. Environmental Protection Agency

Ecosystems Research Division

Center for Exposure Assessment Modeling (CEAM)

960 College Station Road

Athens, Georgia 30605-2700

mailto:ceam@epamail.epa.gov

Software can be downloaded at:

http://www.epa.gov/ceampubl/swater/plumes/

POM	Princeton Ocean Model

Description:
This is a three-dimensional water circulation model which solves for tidal (barotropic) and density (baroclinic) induced flows. The model is one of the most widely-used ocean and shelf circulation model in the world.

Data Requirement:
Boundary and initial conditions for temperature/salinity/density and hydrodynamic forcing functions

Output:
The hydrodynamic outputs from POM are often used to describe the advection and diffusion processes in water quality models. In particular Ecomsed uses POM hydrodynamics in its water quality computations.

Version and System Requirements:
Continually updated and released. Available for DOS/Windows/Unix/LINUX

Assumptions and Limitations:
It does not resolve flows in coastal regions which contain sand banks or mudflats. It may be useful, however, in some Irish coastal waters such as Killary Harbour where significant stratification occurs.

Application History:
The Princeton Ocean Model (POM) was developed originally by Blumberg and Mellor (1987) and has been applied to countless problems. The model is continually being upgraded and refined and is supported via a web-based discussion group.

Availability:
Program in Atmospheric & Oceanic Sciences, P.O. Box CN710, Sayre Hall, Princeton University, Princeton, New Jersey 08544-0710.
POM is freely available to the academic community from PU after registration at: http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/registration.htm

Website:

http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/

PROFILE

Description:
PROFILE facilitates analysis and reduction of in-lake water quality data. Algorithms are included for calculation of hypolimnetic oxygen depletion rates and estimation of area-weighted, surface-layer mean concentrations of nutrients and other eutrophication response variables.

Data Requirement:
Vertical profiles of water quality data collected at one or more sample stations throughout the period of interest.

Output:
Graphic and tabular displays allow users to evaluate and summarize lake or reservoir water quality data. Mixed-layer water quality summaries (means) and hypolimnetic oxygen depletion rates, and associated error statistics (CV) are provided as input to BATHTUB.

Availability:
Distributor: Dr. Robert H. Kennedy

Environmental Laboratory

U.S. Army Engineer Waterways Experiment Station

3909 Halls Ferry Road

Vicksburg, MS 39180

kennedr@wes.army.mil

The model can be downloaded at:

http://www.wes.army.mil/el/elmodels/

Website:

http://www.wes.army.mil/el/elmodels/emiinfo.html

PROTECH Phytoplankton RespOnses To Environmental Control

Description:
At the core of all the models is a series of regression equations which describe the performance of common phytoplankton in controlled laboratory conditions of temperature and insolation in terms of algal cell morphology (Reynolds, 1989; Reynolds & Irish, 1997). Caveats to allow for species-specific traits, such as the capability of certain cyanobacteria to fix atmospheric nitrogen or the additional requirement of diatoms for an adequacy of skeletal silicon, are incorporated. The potential rate of increase for each of up to eight species "seeded" into the model at day 1 is calculated against the temperature and daily insolation obtaining. The model checks that the resource base of nutrients will sustain this and, if so, allows each to increase its biomass accordingly and deducts the nutrients consumed from the resource base. It also allows biomass to be transported out of the water body and it allows algae to be removed by grazing animals. The latter routine adopts the temperature - and food-dependent growth and reproduction relationships developed for Daphnia (Reynolds, 1984). The model assumes that all algae thus consumed return the component nutrients back to the water. At the end of each round of calculations, the new standing population of each species is re-totalled, as is the residue of each nutrient resource and the coefficient of underwater light extinction, as modified by the altered biomass of algae. In this way, the model can simulate reasonable approximations of the growth and attrition phases of phytoplankton in natural lakes, and be realistically sensitive to the effect of season, nutrient supply, grazing and wash-out losses.

Data Requirement:
Physical and chemical seasonal and spatial data, and growth coefficients for algal species.

Version and System Requirements:
A two-dimensional version of PROTECH was developed, called PROTECH2. The model software PROTECH2 was supplied to the NRA as (Reynolds & Irish, 1993 and IFE 1993).

The software of this version remains the property of the Environment Agency and is not in general use.

Later an "accumulating subroutines" to PROTECH2, in an effect to include a layer of bottom sediment to store settling material. It is hoped to develop a recycle facility into PROTECH3 model that better simulates the rapid nutrient turnover of shallow lakes. PROTECH-C has been developed specifically for use in reservoirs where the volumes of water exchanged by surface flow can be supplemented by pumping operations. Moreover, in respect of the fact that there is often as much concern about BOD of the stored water as its algal content, the currency of PROTECH-C models can be changed to organic carbon.

A novel addition to the present model has been the incorporation of the effects of artificial mixing induced by the bubble aeration. This is written into PROTECH-C as an override to subcritical Monin-Obukhov calculations, which otherwise allow stratification to occur.

Assumptions and Limitations:

PROTECH and PROTECH-C can be relied upon only within its own limitations. The PROTECH philosophy has always been geared to the maximum capacities of systems, the worst-case scenarios, as it were. An output to a given level of carbon or chlorophyll assumes that everything introduced into each simulation will perform to its biological best. Early versions do not recognise carbon limitation the supply of CO_2 from the atmosphere and the dissociation of bicarbonate is assumed always to be adequate) and no other element, apart from nitrogen, phosphorus or silicon can be exhausted. Growth limitation by other elements, including carbon, will be incorporated in due course. An inoculum of every alga chosen is preceded everyday, regardless of whether it is actually supplied in the riverine inflow or of whether the last flushing removed all inocula from the water column. The choice of the inoculated species is almost arbitrary - a result in favour of one species does not necessarily imply that it will do so or that others will not.

Website:

http://windermere.ceh.ac.uk/algalmodelling/contents/ProtechC/ProtechCPage.htm

QWASI	***Q*uantitative *W*ater, *A*ir and *S*ediment *I*nteraction**

<u>MODIFIED VERSION FOR EUTOX APPROACH</u>

Description:

QUASI was originally designed to describe the steady state behaviour of an organic chemical in a lake subject to chemical inputs by direct discharge, inflow in rivers, and deposition from the atmosphere. The mass balance equations for the well-mixed water column and the well-mixed layer of surficial sediment also include sediment-water exchange by diffusion, deposition, and re-suspension.

Wania (1996) presented a modified version of QUASI to study the interaction of nutrients and contaminants. The model was parameterised for several typical HOCs in a generic lake and input parameters related to the organic carbon dynamics were adjusted to reflect different trophic conditions.

Most important modifications from original QUASI m odel:

Most important modifications from original QUASI model:

- Inclusion of the atmosphere above the lake as a compartment, the concentration of which is calculated rather than being a model input. This allows for the lake to have an influence on the concentration in the air above the lake, which may be of importance for large lakes and chemicals with large air-water exchange fluxes. The user has to input the background concentration in the air flowing into the lake area.
- Description of the particle-associated transport of HOC on the basis of particulate organic carbon (POC) rather than total solids, and the derivation of the transport parameters for POC settling, re-suspension and burial within the model.
- Calculation of some of the transport parameters describing the atmosphere-water exchange from meteorological and chemical specific data instead of using generic values.
- Programming the model in Stella II-format to facilitate the modelling g of non-steady state scenarios with time-variant input parameters.

Assumptions and Limitations:

The partitioning of HOCs to DOC or colloidal material is not taken into account.

Application History:
Wania (1996) simulated the interactions between HOCs and nutrients in an eutrophic lake and oligotrophic lake.

Availability and Website:
The original version of QWASI is available at:

http://www.trentu.ca/cemc/models/Qwasi.html

RAM

Description:
RAM is a risk assessment based network model. The modelling software allows the user to construct a model incorporating information about the contaminant source site geometry, engineered features, geological formations and hydrogeological conditions, and to predict contaminant migration and fate in the system.

The model is designed to be compatible with risk assessment carried out under the British Environment Agency's (EA) framework of tiered risk assessment for protection of surface- and ground water resources from contamination (Environment Agency, 2000). RAM allows the construction of simple single source, pathway, receptor networks and also more complex networks of multiple sources, pathways and/or receptors through the hydrogeological system in question. Saturated groundwater flow through the system is modelled in one dimension using Darcy's law and water balance equations. Unsaturated flow is modelled using a water balance approach. The processes that can be modelled for each contaminant across the hydrogeological units defined in the pathway are: Derivation of source pore water concentrations from soil concentrations, (corresponds to EA Tier 1 assessment for single source, pathway, receptor networks); Dilution processes (with Tier1 corresponds to EA Tier 2 assessment for single source, pathway, receptor networks) Advection, Dispersion, Retardation and Decay (with Tier 2 corresponds to Tier 3 assessment for single source, pathway, receptor networks) Tier 4 assessment corresponds to Tier 3, but for more complex multiple source, pathway and/or receptor networks.

RAM is integrated with the Crystal Ball software for probabilistic risk assessment. Transient simulations can be carried out, by specifying a single storage parameter for the simulation. Results are then reported for the specified time slices.

Data Requirement:
See chapter 5.10, section **'*Data Requirements for Network Models for contaminant transport'.***

Output:
Results from the model consist of, for each pathway, contaminant species and timeslice: concentration at the receptor, remedial concentrations at the source, dilution and attenuation factors for the pathway. Probabilistic simulations will produce the same set of results but at the percentile specified for the model simulation.

Version and System Requirements:
Ram Version 1 is most recent version

System Requirements: PC Pentium, at least 64 Mb RAM and 10 Mb of hard-disk space

O.S.: Windows, 95, NT, 98, 2000

Assumptions and Limitations:
See chapter 5, section 5.10, *'Network Models for Contaminant Transport'*.

Application History:
A relatively new model, but robust and with very useful features, well implemented. Also ESI Ltd. traditionally produce good modelling software.

Availability and Website:
Developed by and available to order online from Environmental Simulations Limited at:

http://www.groundwatermodels.com/software/SoftwareDesc.asp?software_desc_id=75&software_id=10

REGCEL	**Water level analysis**

Description:
REGCEL is a water level analysis tool developed for application to the lakes of Finland by the Finnish Environment Institute. Ecological impacts are indicated by the severity of change in a number of ecologically relevant aspects of the water level regime, e.g. seasonal maximum water levels, maximum summer water level fluctuation, water level at time of annual thaw (Hellsten *et al*., 2002).

Data Requirement:
Daily water levels are used, and are required for both un-impacted and impacted conditions for the same water body – continuous data over many years are preferred.

Output:
Qualitative indications of ecological impact

Version and System Requirements:
Requires MS Excel

Assumptions and Limitations:
Recalibration work will be required for application to Irish waters

Availability:
Contact author: Dr Seppo Hellsten – mailto:seppo.hellsten@ymparisto.fi

Dr Mika Marttunen - mailto:Mika.Marttunen@ymparisto.fi

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RHABSIM Riverine HABitat SIMulation

Description:
RHABSIM is a fully integrated program for river hydraulics and aquatic habitat modelling using the Instream Flow Incremental Methodology (IFIM). Running in Microsoft Windows and DOS, it is an extensive conversion of the PHABSIM hydraulic and habitat simulation system developed by the U.S. Fish and Wildlife Service.

Data Requirement:
Field data entry: Easy data input and integrity checking; Full implementation of Cross-section raw data entry.
Import and export PHABSIM data files (IFG4, MSQ and WSP): Import standard ASCII files with X, Y, Vel and Attribute data; Import acoustic Doppler files.

Version and System Requirements:
- PC with 486 or Pentium CPU.
- VGA or SVGA graphics card.
- Operating system: Windows 3.1, Win95 or Win98.
- Required minimum disk space: 6 mb.
- minimum memory: 16 mb.

Assumptions and Limitations:
RHABSIM data files and processing allow the following data limits:
- Up to 100 cross-sections per data file.
- Up to 300 data points per cross-section.
- Up to five Stage/Discharge calibration sets.
- Up to 30 Calibration Flows (HYDSIM) and Simulation Flows (HABSIM).
- One or two Attribute variables.
- Criteria (species) curves may contain four variables (velocity, depth and two Attributes) and 200 data points.
- Criteria curve library files may contain up to 50 curve sets.
- Habitat simulation production runs may include up to 50 species (curve sets), although a maximum of 10 are used in the Compare runs module.

Time Series data files and production run parameters may contain:

- Up to 600 streamflow columns (50 years as daily data).
- Up to 10 Flow Releases.
- Up to 20 Exceedence Percentiles to report (although all 99 may be reported).
- Weighted Usable Area data may have up to 30 flows and ten species (criteria curves).

Availability:
The RHABSIM full package Single User License currently costs $895 (U.S. funds). The license entitles you to one year technical support (via phone and/or e-mail) and one ***free upgrade*** to new release. Registered users will also receive a discount on future upgrades and new version releases.

Orders can be placed electronically at: http://www.northcoast.com/~trpa/order.html

Contact:

Thomas R. Payne and Associates

890 L Street, Arcata, California USA 95521

P.O. Box 4678, Arcata, California USA 95518

(707) 822-8478

Website:
http://www.northcoast.com/~trpa/

RHS **River Habitat Survey**

Description:

"River Habitat Survey"(RHS) is a standard method for capturing data on the physical habitat of rivers. RHS was developed to describe and evaluate physical habitat at national, catchment and lesser scales in England, Scotland, Wales and Northern Ireland. It has been applied to in the order of 20,000 sites in the United Kingdom and elsewhere. It is accepted as a standard method for assessing "hydromorphology" to support the European Water Framework Directive. The analysis of RHS data has been used to support rationales for systematically selecting sites for rehabilitation at a catchment scale.

The RHS uses the physical structure of streams to assess the character and quality of rivers. Statistical theory is used to aid the survey design and the selection of sampling sites throughout the U.K. (Jeffers, 1998b, Fox *et al*., 1998). At each randomly selected site, a 500m length of river is surveyed. At 50m intervals along this length of river, 10 spot checks are performed. A range of features is recorded at each spot check. To ensure that features and modifications not occurring at the spot checks are included, a sweep up checklist is also completed (Raven *et al*., 1998b). In addition, cross sectional measurements of water and bankfull width, bank height and water depth are made at one representative location within the 500m sampling site (Raven *et al*., 1998b). When used in conjunction with the survey data, these measurements provide information about the geomorphological processes acting on the site (Raven *et al*., 1997). Variables such as altitude, slope, planform and geology derived from maps. Data are entered onto an electronic database and photos of each sampling site are also stored electronically (Raven *et al*., 1998b).

RIVPACS **River InVertebrate Prediction And Classification System**

Description:
In the early 1980s the Water Authorities in Britain identified the need for a greater understanding of the variation in running water sites and their macroinvertebrate communities. It was realised that such information was fundamental to the development of a nationwide biological assessment programme. A long-term project was established to develop a biological classification of unpolluted running water sites in Great Britain based on the macroinvertebrate fauna and then to create a system whereby the macroinvertebrate community at a site could be predicted using physical and chemical features. This initiative led to the development of the RIVPACS type approach to biological assessment by the River Communities Group at the Centre for Ecology and Hydrology (CEH), which has subsequently been adopted by other countries and forms the basis of the European Union Water Framework Directive (European Commission, 2000). RIVPACS is the resultant software package to assess the biological quality of rivers and streams in the United Kingdom. Equivalent software packages have also been developed in other countries where the generic RIVPACS type approach (also termed reference condition approach) has been applied. In 1997 a major International conference was held in Oxford University to present and discuss the various methodologies of bioassessment of freshwater bodies that had been developed or were being developed around the world. The conference focussed mainly on RIVPACS type systems but also included multi-metric and artificial intelligence approaches.

Data Requirement:
When a fully validated RIVPACS type predictive model has been developed for a region or country, it can then be used to assess the ecological status of new running water sites of unknown quality. At these new test sites a biological sample is collected and the relevant physicochemical variables measured using the same standard protocols as were used for the reference sites. The RIVPACS predictive model then generates an Expected Fauna from the measured environmental variables. Biotic indices are calculated from this list of expected taxa. The biological sample taken at the test site provides an Observed Fauna from which biotic indices are also calculated.

The Expected and Observed values for various biotic indices are then compared using Environmental Quality Indices (EQI). These are values derived from the ratio of Observed: Expected. The higher the EQI value the closer the observed fauna matches that expected at the site in the absence of any environmental stress.

Output:
The RIVPACS type model will provide an output consisting of observed and expected faunal lists (perhaps with expected abundances), observed and expected biotic index values and associated EQI values. The EQI values can be banded into quality classes to aid interpretation of the data across the entire region or country.

Version and System Requirements:
The version RIVPACS III+ includes a reference site classification system. There are 35 classification groups in the Great Britain module and 11 classification groups in the Northern Ireland module.

Assumptions and Limitations:
Errors in estimates of the expected fauna are potentially due to:

- Having an inadequate set of reference sites; too few or poor coverage of some stream types.
- Although all of good or high quality, the reference sites are not all of the same quality. In fact they will vary considerable in quality, however biological quality is defined.
- The macroinvertebrate data for the references sites will be subject to the usual effects of sample variation.
- Not involving all relevant environmental variables (e.g. macrophyte or habitat diversity). The best environmental variables for predicting fauna may include some, such as chemistry or current flow that are a cause of the stress or pollution which the RIVPACS model is trying to assess. It is important to try to exclude such variables. Essentially a predictive model is needed which is "fit for purpose".
- Not making optimum predictive use of variables.
- Errors in measuring the environmental variables for new test sites from which predictions of their expected fauna are made.

Application History:

Freshwater ecologists CEH in the UK pioneered the RIVPACS type approach. However it has been trialled, and in some cases adopted, in many countries seeking to establish a national or regional freshwater bioassessment scheme.

The Australian River Assessment Scheme (AUSRIVAS) was developed during the 1990s in response to a greater awareness of the threats to Australian freshwater ecosystems. AUSRIVAS is based on a RIVPACS type approach but inevitably has a number of distinct features from the UK RIVPACS model. There are individual AUSRIVAS models specific to each region's macroinvertebrate fauna and environmental conditions, which increases the predictive accuracy of the scheme overall.

Environment Canada (National Water Research Institute and Ontario Region) has developed a RIVPACS type approach to assess freshwater sediments in the near-shore areas of the Great Lakes. Preliminary RIVPACS type models have been constructed for some watersheds in the US and there has been a recent influential study by US biologists that evaluated the use of a RIVPACS type approach and they concluded that the approach is very effective, is based on sound scientific principles and they strongly urged that it should be evaluated elsewhere in the US. Ultimately they see multimetric and RIVPACS type approaches as complementary. Changes to New Zealand legislation in the early 1990s shifted the emphasis of water management from chemical water quality to the broader assessment of aquatic ecosystem health. Macroinvertebrate-based indices are currently used in the routine monitoring of rivers and streams but recently there have been successful pilot studies using the RIVPACS type approach within certain regions or water sheds. Indeed the approach has been applied to fish and macro-crustaceans as well as macroinvertebrates. The RIVPACS type approach had considerable influence on the drafting of the Directive. The core concept of the WFD, that an ecological status target is set for each site, is essentially derived from the RIVPACS type approach. These targets are based on a fundamental knowledge of the relationship between the biota and the physicochemical environment and involve the definition of the 'Reference Condition' for each test site. The WFD requires that all water bodies are classified into groups of similar type, based on a range of environmental variables. This is also adapted from the RIVPACS methodology.

Availability:

The software is available from

Centre for Ecology and Hydrology,
CEH Dorset, Winfrith Technology Centre,
DORCHESTER, Dorset DT2 8ZD, UK
Contact: Ralph Clarke
Email: rtc@ceh.ac.uk
Tel No: 00 44 (0)1305 213500
Fax No: 00 44 (0)1305 213600

Website:

http://www.dorset.ceh.ac.uk/our_science/General Sections/waterquality/Rivpacs_2003/rivpacs_introduction.htm

RZWQM Root Zone Water Quality Model

Description:

The RZWQM has been developed of the past ten years by a team of ARS scientists. A majority of the team members are part of the present Great Plains Systems Research Unit, Fort Collins, CO. Recently, some parts of the model have been revised and enhanced with cooperation of the ARS Northwest Watershed Research Laboratory, Boise, ID, and the ARS Nematode Research Laboratory, Tifton, GA.

Root Zone Water Quality Model (RZWQM) simulates major physical, chemical, and biological processes in an agricultural crop production system. RZWQM is a one-dimensional (vertical in the soil profile) process-based model that simulates the growth of the plant and the movement of water, nutrients and agro-chemicals over, within and below the crop root zone of a unit area of an agricultural cropping system under a range of common management practices. The model includes simulation of a tile drainage system.

Data Requirement and Output:

RZWQM consists of six major scientific submodules or processes that define the simulation program, a Numerical Grid Generator, and an Output Report Generator. Interaction between these programs is achieved through the use of seven input datafiles and three generated output files. The user can create and modify input files using a commercial editor. The model generators three general output files with twenty-five optional debugging output files that provide detailed results generated by the model. The Output Report Generator uses model results to create summary tables and publication quality graphical output in 2- and 3-dimensional formats. The most recent version of the model will have a Windows 95 user interface.

Version and System Requirements:

80386 or better CPU based computer with math coprocessor

Hard disk with at least 10 megabytes free space

Floppy disk drive capable of reading high density formatted disks (5-1/4" or 3-1/2")

MS-DOS operating system (Ver. 5.0 or later)

At least 4 megabytes of RAM with 640 kilobytes of conventional memory

Graphic display card (VGA, EGA, or better).

Assumptions and Limitations:

The crops parameterised are limited to corn, soybean and wheat.

Both input and output are in metric units.

The complexity of the processes and the need to interpret model results favour the technical staff of most agencies as model users.

Frozen soil dynamics are not considered.

Rainfall is entered as break point increments

A fairly detailed description of the soil profile and initial state has to be known to give good simulation response for the system.

Availability:

Contact:

Laj Ahuja

USDA, ARS, Great Plains Systems Research Unit, P.O. Box E, 301 S. Howes, Fort Collins, Colorado 80522

Phone: (970) 490-8315

Fax: 970)490-8310

email: ahuja@gpsr.colostate.edu

Kenneth Rojas

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The model can be downloaded at:

http://arsagsoftware.ars.usda.gov/rootzone/registra.htm

Website:

http://gpsr.ars.usda.gov/products/rzwqm.htm

SED3D Three-Dimensional Numerical Model of Hydrodynamics and Sediment

Description:
The Three-Dimensional Numerical Model of Hydrodynamics and Sediment Transport in Lakes and Estuaries (SED3D) simulates the flow and sediment transport in lakes, estuaries, harbours, and coastal waters. SED3D is a dynamic modelling system that can be used to simulate the flow and sediment transport in various water bodies under the. This model can be run in a three-dimensional mode, a two-dimensional vertically integrated 'x-y' mode, or a two-dimensional 'x-z' mode. The model contains a free-surface, as opposed to a rigid-lid, with proper boundary conditions for velocity, temperature, salinity, and sediment. A simplified second-order closure model of turbulent transport is used to compute the vertical eddy viscosity and diffusivity contained in the model equations.

Data Requirement:
Boundary hydrodynamics and climatology, freshwater inflows, density gradients and sediment characteristics.

Output:
Given proper boundary and initial conditions, the model can compute the time-dependent, three-dimensional velocity components (u,v,w), temperature (T), salinity (S), and suspended sediment concentration (C) in the Cartesian and vertically stretched grid system (x,y,s).

Version and System Requirements:
DOS or VAX based. Only at Beta release stage.

Application History:
Only at test stage

Availability and Website:
U.S. Environmental Protection Agency, Ecosystems Research Division, Center for Exposure Assessment Modelling (CEAM), 960 College Station Road, Athens, Georgia 30605-2700.

The model can be downloaded at:

http://www.epa.gov/ceampubl/swater/sed3d

SHE — Système Hydrologique Européen

Description:

The SHE model has been developed by the joined efforts of the British Institute of Hydrology, the Danish Hydraulic Institute and the French consulting company SOGREAH. The hydrological processes are modelled by finite difference representations of the partial differential equations for the conservation of mass, momentum and energy and completed by empirical equations (Abbot *et al*., 1986a).

The major physical processes (components) represented by the model are:

- - snow melt- overland flow
- - canopy interception- unsaturated flow
- - evapotranspiration - saturated flow
- channel flow

Data Requirement:

Input variables for physical components are : rainfall rate; precipitation; meteorologic data; flows or water levels at boundaries; man controlled flows and diversions; flows or potentials at boundaries and pumping and recharge data.

Version and System Requirements:

Models such as SHE use of large arrays of data and involve extensive iterative numerical solution techniques. These models thus require very large amounts of computation time and memory. For practical applications, mainframe computers are still needed for running these models.

Assumptions and Limitations:

A fundamental problem with relation to this type of models relies in the fact that the physical approach based on the use of differential equations will yield satisfactory results only when the initial and boundary conditions are set accurately.

A second fundamental problem is related to the discretisation of both time and space. If it is desirable to increase the grid spacing and time step as much as possible in view of minimising data inputs and computation time, the numerical techniques and the nature of the psychical processes require relatively small increments. A typical example of a component that will require small increments is the groundwater flow near the rivers, where strong water level gradients prevail. Considering the time discretisation, it is also important to consider the difference in the characteristic time-base of the processes involved (e.g. fast surface runoff vs. slow groundwater flow). The discretisation problem has been proven to be a very sensitive one

Availability:

Contact:

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SMIC Surface Water and Water Quality Models Information Clearinghouse

Description:
SMIC is a database of the descriptions and features of environmental surface water and water quality models, and abstracts of projects using those models. The interactive features of this website are designed to help in choosing a model for a particular application, and in making comparisons between models.

Availability:
Links to archives of models and modelling tools are available at:

http://smig.usgs.gov/SMIG/model_archives.html

Website:
http://smig.usgs.gov/SMIC/SMIC.html

SOBEK

Description:

Water systems are influenced by many different factors. Heavier than expected rainfall, high winds and pollution loads can have an impact on the water system. SOBEK 's integrated format is designed to check effectiveness of measures taken to keep systems, running at peak efficiency. The designers claim that manual or automatic operation of pumps, sluice gates, weirs, storage tanks and other structures can all be incorporated into the model, giving a realistic picture of how the system behaves in extreme scenarios. Results are displayed as maps, graphs, tables and animations helping analysis and communicating of ideas. SOBEK has three basic product lines covering fresh water management situations in River, Rural and Urban systems. Each product line consists of different modules to simulate particular aspects of the water system. These modules can be operated separately or in combination. The data transfer between the modules is fully automatic and modules can be run in sequence or simultaneously to facilitate the physical interaction. SOBEK has been developed by WL | Delft Hydraulics in partnership with the National Dutch Institute of Inland Water Management and Wastewater Treatment (RIZA), and the major Dutch consulting companies.

Application areas

SOBEK-Rural Irrigation construction, rehabilitation, modernization Drainage and flood protection:

- Long-term and real-time operation of multiple reservoirs
- Real-time control and automation of canal system

SOBEK-Urban Determination of urban drainage capacities, including treatment plants:

- Assessment of sewer overflow frequency
- Design of detention basins
- Real-time control of urban drainage systems
- Environmental study on receiving waters

SOBEK-River Navigation:

- Flood protection, flood-risk assessment
- Water pollution studies

- Estuaries with fresh and salt water
- Sand mining, sediment and morphology studies

The integrated approach provides a instrument for flood forecasting, navigation, optimising drainage systems, controlling irrigation systems, reservoir operation, sewer overflow design, ground water level control, river morphology regulation, and water quality control. The integrated approach also means that SOBEK can combine river systems, urban systems and rural systems.

Version and System Requirements:

The software is available for Windows 95/98 and Windows NT 4.0 platforms. Network versions are available on request. For normal applications SOBEK needs at least 100 Mb of free disk space and a Pentium II processor with 64 Mb memory. For optimal performance a Pentium III processor, 128 Mb memory, and 1 Gb of free disk space is recommended.

Availability and Website:

More information about SOBEK and demonstration versions can be downloaded at: www.sobek.nl

SOIL	Simulation model for soil water movement and heat SOIL-
SOIL-N	Simulation model for nitrogen conditions in soils

Description:
The SOIL model was developed to simulate water and heat processes in soils. It was designed to: assess the importance of different ecological factors; identify gaps in the present knowledge; formulate new hypotheses; generalize results to new soils, climates and time periods; predict the influence of human management, such as soil heat extraction, mulching, drainage, irrigation and plant husbandry and simulate regulating factors for biological and chemical processes in the soil. It was initially developed to simulate water and heat processes in forest soils. Due to several extensions it is now applicable to any soil independent of plant cover which was possible since the model is based on well known physical equations.

The basic structure of the model is a depth profile of the soil, so that the vegetation covered soil is divided into a maximum of 22 layers. Processes such as snow-melt, interception of precipitation and evapotranspiration are examples of important interfaces between soil and atmosphere. Two coupled differential equations for water and heat flow represent the central part of the model. These equations are solved with an explicit numerical method. The basic assumptions behind these equations are the law of conservation of mass and energy and the fact that flows occur as a result of gradients in water potential (Darcy's law) or temperature (Fourier's law).

SOIL can be applied to simulate the heat and water processes in nearly any kind of soil. In coupling it with other models (for example SOILN from the same author) SOIL can be used at a wide range of questions concerning the interactions between nitrogen, soil water and heat, plants, climate and human interventions.

The SOILN model was designed to simulate transport and transformations of nitrogen in soils and its uptake by plants. It was designed by the same author as the SOIL model, of whom SOILN is dependent. It uses some of the SOIL output data as input. SOILN includes the following processes: mineralisation of humus; mineralisation/immobilization of carbon and nitrogen fraction in crop residue and the manure; nitrification; denitrification; nitrate leaching; plant uptake.

Nitrogen treatment by plants depends on the plants.

Therefore two submodels exist, CROP by Eckersten & Jansson (1991) and FORESTSR, which simulate the processes within the plants either for crops (CROP) or trees (FORESTSR). In SOILN this fraction is stored in the compartment N_{plant}.

The soil mineral nitrogen pools receive nitrogen by mineralisation of litter and humus, nitrification, fertilization and deposition and loose nitrogen by immobilization to litter, nitrification, leaching, denitrification and plant uptake. It is also influenced by vertical redistribution. All biological processes depend on soil water and temperature conditions. The soil is divided into layers from which plants are taking nitrogen in various rates. Leaves take up carbon as Roots take up the nitrogen. The leaf area captures the necessary radiation for the photosynthesis. The actual growth of the plants is the potential growth, which is proportional to the intercepted radiation, reduced by the different stresses. The nitrogen demand of the plants is proportion

Availability:

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http://amov.ce.kth.se/AMOVNew.htm#5

SPARROW

Description:
The SPARROW method uses spatially referenced regressions of contaminant transport on watershed attributes to support regional water-quality assessment goals, including descriptions of spatial and temporal patterns in water quality and identification of the factors and processes that influence those conditions. The method is designed to reduce the problems of data interpretation caused by sparse sampling, network bias, and basin heterogeneity. The regression equation relates measured transport rates in streams to spatially referenced descriptors of pollution sources and land-surface and stream-channel characteristics. Spatial referencing of land-based and water-based variables is accomplished via superposition of a set of contiguous land-surface polygons on a digitzed network of stream reaches that define surface-water flow paths for the region of interest. Water-quality measurements are obtained from monitoring stations located in a subset of the stream reaches. Water-quality predictors in the model are developed as a function of both reach and land-surface attributes and include quantities describing contaminant sources (point and nonpoint) as well as factors associated with rates of material transport through the watershed (such as soil permeability and stream velocity). Predictor formulae describe the transport of contaminant mass from specific sources to the downstream end of a specific reach. Loss of contaminant mass occurs during both overland and in-stream transport. In calibrating the model, measured rates of contaminant transport are regressed on predicted transport rates at the locations of the monitoring stations, giving rise to a set of estimated linear and nonlinear coefficients from the predictor formulae. Once calibrated, the model is used to estimate contaminant transport and concentration in all stream reaches. A variety of regional characterizations of water-quality conditions are then possible based on statistical summarization of reach-level estimates. The application of bootstrap techniques allows estimation of the uncertainty of model coefficients and predictions.

Website:
http://water.usgs.gov/nawqa/sparrow/intro/intro.html

STONE

Description:
The STONE model is a joint product of several research institutes in the Netherlands. The aim of STONE is to predict the current and future emission of nitrogen and phosphorus to surface and groundwater. The model consists of three sub-models. First, the CLEAN sub-model calculates the distribution of manure across the Netherlands and the emission of nutrients towards soil and air (*i*). Second, the OPS/SRM submodel calculates the deposition of nitrogen from the atmosphere resulting from agricultural and secondary sources (*ii*). Finally, the ANIMO submodel, which is incorporated in a geographical shell (GONAT (*iii*)), computes the emission of nutrients towards both groundwater and surface water. In ANIMO, the nutrient uptake by the crops is calculated by the QUADMOD module. This chain of models is accessed by a graphical user interface. This interface allows the user to change the model scenarios, run the model and view the model outputs. STONE is provided with a large set of fixed data, such as the hydrological data which are calculated separately by the SWAP model. These fixed data are considered boundary conditions for STONE. Since spatial and temporal resolutions of the three sub-models are different, conversion programs are included.

Main Function, Data Requirement and Data Output:
Model chain of STONE:

<u>CLEAN</u>
Calculates emission of ammonia from agricultural sources; Calculates annual supply of N and P in manure to the soil; Modelling of manure production and distribution; Linear programming model for optimised allocation of manure; Number of animals; Excretion per animal; Fraction of Ammonia; Volatilisation; Partitioning of animals over stable types; Fertilizer recommendations; Areas with crop/soil comb; Manure application per region; Inorganic Fertilizer appl. per region; Manure transfer to other regions; Manure surplus or appl. capacity and Ammonia emission

<u>OPS/SRM</u>
Calculates deposition of ammonia; Matrix of relationships between emission and deposition as based on results from statistical atmospheric transport model Ammonia emission and Ammonia deposition

SWAP

Calculates vertical transport of water in unsaturated and saturated layers of soil; Complex deterministic agro-hydrological model; Meteorological data; Irrigation data; Crop characteristics; Cropping calendar; Soil water and hydraulic characteristics; Drainage characteristics; Components of water balance; Soil moisture profile over time; Soil temperature profile; Water fluxes to/from surface water; Groundwater-level and Crop growth.

GONAT/ANIMO

Calculates nutrient fluxes to surface water; Calculates nutrient fluxes to ground water; Calculates phosphorus loading of soils; Complex deterministic N and P cycling and leaching model; Water fluxes per layer Inorganic and organic fertilizer application; Nutrient deposition Soil chemical, sorption, precipitation and conversion characteristics

Decomposition and N and P mineralisation characteristic. Crop N and P uptake; N and P fluxes to the different Drainage systems (i.e. canals, ditches, tile drains); N and P fluxes to deeper groundwater; Adsorption of phosphate Precipitation of phosphate; N balance; P balance and Change in organic N and P.

QUADMOD

Calculates nutrient uptake and yield; Empirical model; Soil nutrient supply Fertilizer application Empirical parameters as based on field trials.

Assumptions and Limitations:

The start of the simulations is on January 1 st 1986. All scenarios follow a simulation period of multitudes of 15 years. Two hydrological data sets are available, one for the period 1971-1985 and one for the period 1986-2000. Therefore, when projections are made for the year 2005, the hydrological situation of either 1975, or 1990 is used. Because the hydrological data are available on a daily basis, the effects of variability of weather can be taken into account.

Application History: The STONE model consists of several submodels, which have been validated independently. The STONE model results on the emission of nitrogen and phosphorus towards groundwater and surface waters in the Netherlands. These results are used for formulating environmental policies and may have potentially severe economical, environmental, social and jurisdictional impact of eutrophication abatement plans. Therefore it is important that the STONE system as a whole is validated. The validation study consists of several stages. In a first stage, the model is compared with lumped observations from both groundwater and surface water monitoring networks. This stage will give general information about model behaviour vis-à-vis real world data at the (aggregated) target scale level. Since October 2001 further model testing, validation and uncertainty analysis of the model chain as a whole is being carried out. **Website:** http://www.alterra.nl/models/stone/p_stone_model.htm

SWAT	Soil and Water Assessment Tool

Description:
SWAT is a continuous time model that operates on a daily time step at basin scale. The objective of such a model is to predict the long-term impacts in large basins of management and also timing of agricultural practices within a year (i.e., crop rotations, planting and harvest dates, irrigation, fertilizer, and pesticide application rates and timing). It can be used to simulate at the basin scale water and nutrients cycle in landscapes whose dominant land use is agriculture. It can also help in assessing the environmental efficiency of BMPs and alternative management policies.

Data Requirement:
Main model input (sensitive) parameters:

A) Soil Map. For each soil layer:

-Textural properties:

- Physico-chemical-properties:

B) Land use Map

Land use information: crop, water bodies (lake, pond, etc.)

Cropping information: planting and harvest date, yield, etc.

Management practices: fertilizer and pesticide application timing and amount

C) Climate Information

Daily rainfall, minimum and maximum air temperature, net solar radiation

Monthly average wind speed

Average monthly humidity

D) Water Quality Information

F) Point sources

- Location

- average daily flow

- average daily sediment and nutrient loading

G) Hydrogeological Map

Groundwater abstraction timing and amount

H) Digital Elevation Model

I) Monitoring Data for model calibration:

- Observed flows at sub-basin /basin outlet(s)

- Nutrient loadings at sub-basin/basin outlet (s)
- Sediment loadings at sub-basin/basin outlet(s)

Version and System Requirements:
SWAT94.2, SWAT 96.2, SWAT98.1, SWAT99.2, SWAT2000

Assumptions and Limitations:
This model subdivides large river basins into homogenous parts, then analyses each part and its interaction with the whole. SWAT is spatially distributed, so that these parts can interact. The model simulates hydrology, pesticides and nutrient cycling, erosion and sediment transport. Input consists of files, information from databases and information from GIS interface. More specific information can be entered singly, for each area or for the watershed as a whole.

Availability:
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Websites:

SWAT Website

http://www.brc.tamus.edu/swat/

SWAT Documentation

http://www.brc.tamus.edu/swat/swatdoc.html

Hydrologic Unit Model for the U.S. (HUMUS)

http://srph.brc.tamus.edu/humus

SWAT User's Group

mailto:Subscribe swat-request@blacklandgrass.tamu.edu

Post Message mailto:swat@blacklandgrass.tamu.edu

SWIM	Soil and Water Integrated Model

Description:

SWIM was developed in the Potsdam Institute for Climate Impact Research on the basis of two other models: SWAT (Arnold *et al*., 1993 & 1994) and MATSALU (Krysanova *et al*., 1989). The SWAT model was developed in the Blackland Research Center (USDA ARS, Temple, Texas) to predict the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds with varying soils, land use and management conditions. To satisfy this objective, the model is process-based, uses readily available inputs, is computationally efficient, and enables users to study long-term impacts. SWAT incorporates features of several ARS models and is a direct outgrowth of the SWRRB model. Specific models that contributed significantly to the development of SWAT were CREAMS, GLEAMS, and EPIC. The MATSALU model developed in Estonia on the basis of CREAMS has the similar structure as SWAT.

The model SWIM was developed with an intention to incorporate the best features of both SWAT and MATSALU and to be transferable to other basins in Europe. During the last three years SWIM was extensively tested and validated in a number of mesoscale basins in Germany (mainly belonging to the Elbe river drainage area) regarding different processes – hydrological, vegetation, nutrients and erosion. Though still SWIM has many common modules with SWAT, there are certain essential differences, like the three-level spatial disaggregation scheme implemented in SWIM, a new water routing routine based on the Muskingum method, and a new method for the adjustment of net photosynthesis and evapotranspiration to higher CO2. Besides that, validation of SWIM with the daily time step is an advantage in comparison with SWAT, which is usually validated only with monthly and annual time steps.

Data Requirement:

Climate data, hydrological data, soil base data, crop management parameters

Website:

http://www.brc.tamus.edu/swat/othermod/swim-des5p.htm

SWMM **Storm Water Management Model**

Description:
This programme simulates rainfall, runoff, transport, and water quality processes in urban and some non-urban catchments. Both single storm event and continuous simulation may be used to characterise the response of catchments to inputs of precipitation and related meteorological time series. Flow in open channels and closed conduits may be simulated.

The Runoff Block converts precipitation, from one or more gages, to runoff using a non-linear reservoir method, with infiltration losses based on the Horton or Green-Ampt equations. Water that infiltrates may be optionally routed through groundwater storage. Continuous moisture accounting is performed, and snowmelt may be simulated as well as infiltration/inflow and many other options. Up to a few thousand subcatchments and channel/pipes may be used to discretise the overall catchment.

Other functions include flow and quality routing in channels and conduits; backwater effects, reverse flow, looped connections, surcharging, pressure flow, weirs, orifices, culverts, pumps, time-variable regulator settings and storage routing. Natural channel sections, bridges, and best management practices as well as other options may be simulated.

Data Requirement:
Input data include: historic or synthetic long-term or single-event precipitation hyetographs and optional ancillary meteorological time series such as evaporation and wind speeds; catchment topography, imperviousness, shape factor, depression storage, Manning roughness, and infiltration parameters; optional data for simulation of groundwater flow, snowmelt, infiltration/inflow etc.; channel/pipe and drainage network information. Input for the basic EPA Fortran engine must be prepared in the form of input data files using a standard text editor.

Output:
Output is in the form of hydrographs, pollutographs (concentration vs. time), and time series of other state variables such as stages, volumes and loads, and in the form of statistical summaries. Various continuity checks are performed.

Version and System Requirements:
The program is developed for MS-DOS or Microsoft Windows-based (95/98/NT) microcomputers. The program runs best in a fast Pentium environment. It is written in Fortran 77 with some extensions to Fortran 90. Minimum storage of about 20 Mb is required. The basic Fortran engine is in the public domain. Source code is provided.

An updated beta test version (B) of SWMM 5 is available from the USEPA for evaluation at: http://www.epa.gov/ednnrmrl/swmm/beta_test.htm

The official version of SWMM 5, scheduled for release in October 2003, will include the final QA/QC report and complete documentation in the form of a Users Manual, a Tutorial Help file, a Reference Manual, and a Programmers Manual

Application History:
Extensive. Although used primarily in the United States and Canada, a world-wide user base exists of several thousand engineers, since 1971.

Availability and Websites:
Center for Exposure Assessment Modeling (CEAM)

National Exposure Research Laboratory - Ecosystems Research Division

Office of Research and Development (ORD)

U.S. Environmental Protection Agency (U.S. EPA)

960 College Station Road

Athens, Georgia (GA) 30605-2700

Voice phone: (706) 355-8400

The program may be downloaded directly from the CEAM web page. Additional EPA programs are also available on the CEAM web site, beginning at: http://www.epa.gov/ceampubl/ or

http://ccee.oregonstate.edu/swmm/

SWRRB Simulator for Water Resources in Rural Basins

Description:

SWRRB was developed by Williams *et al.* (1985), and Arnold *et al.*, (1990) for evaluating catchment scale water quality. SWRRB operates on a daily time step and simulates weather, hydrology, crop growth, sedimentation, and nitrogen, phosphorous, and pesticide movement. The model was developed by modifying the CREAMS (Knisel, 1980) daily rainfall hydrology model for application to large, complex, rural catchments. Surface runoff is calculated using the Soil Conservation Service Curve Number technique. Sediment yield is computed for each catchment by using the Modified Universal Soil Loss Equation (Williams and Berndt, 1977). The channel and floodplain sediment routing model is composed of two components operating simultaneously (deposition and degradation). Degradation is based on Bagnold's stream power concept and deposition is based on the fall velocity of the sediment particles. Return flow is calculated as a function of soil water content and return flow travel time. The percolation component uses a storage routing model combined with a crack flow model to predict the flow through the root zone. The crop growth model (Arnold *et al.*, 1990) computes total biomass each day during the growing season as a function of solar radiation and leaf area index. The pollutant transport portion is subdivided into one part handling soluble pollutants and another part handling sediment attached pollutants. The methods used to predict nitrogen and phosphorus yields from the rural catchments are adopted from CREAMS (Knisel, 1980). The nitrogen and phosphorus calculations are performed using relationships between chemical concentration, sediment yield and runoff volume. The pesticide component is directly taken from Holst and Kutney (1989) and is a modification of the CREAMS (Smith and Williams, 1980) pesticide model. The amount of pesticide reaching the ground or plants is based on a pesticide application efficiency factor. Empirical equations are used for calculating pesticide washoff which are based on threshold rainfall amount. Pesticide decay from the plants and the soil are predicted using exponential functions based on the decay constant for pesticide in the soil, and half life of pesticide on foliar residue.

Data Requirement:

Meteorologic data comprising of daily precipitation and solar radiation are required for hydrology simulations. In addition information is required on soils, land use, fertilizer and pesticide applications.

Output:

The model estimates daily runoff volume and peak rate, sediment yield, evapotranspiration, percolation, return flow, and pesticide concentration in runoff and sediment.

Version and System Requirements:

The SWRRB program is written in standard FORTRAN 77 and has been installed on IBM PC/AT and compatibles. A hard disk is required for operation of the program and a math co-processor is highly recommended.

Assumptions and limitations:

Snow accumulation processes are ignored, and for the case of pesticides no comprehensive instream simulation isdone. Nutrient transformations along with pesticide daughter products are not simulated

Application History:

The SWRRB model has been used by the Exposure Assessment Branch, Hazard Evaluation Division, and the Office of Pesticide Programs of the USEPA. SWRRB was tested on 11 large catchments by Arnold and Williams (1987). These catchments were located at eight Agricultural Research Service locations throughout the United States. The results showed that SWRRB can realistically simulate water and sediment yield under a wide range of soils, climate, land-use, topography, and management systems.

Availability:

For copies of the SWRRB program and the user manual contact:

USDA, ARS

Nancy Sa*mmons*

808 East Blackland Road

Temple, Texas 76502

(817) 770-6512

mailto:sammons@brcsun0.tamu.edu

Website:

http://abe.www.ecn.purdue.edu/~wepphtml/wepp/wepptut/jhtml/swrrb.html

TELEMAC	Numerical modelling system for free surface hydrodynamics, sedimentology, water quality, waves and underground flows

Description:
Using finite element techniques, TELEMAC solves the shallow water equations, either vertically averaged in two dimensions or layered in three dimensions. Using unstructured triangular grids, boundary conditions can be applied away from areas of interest, which in turn can be modelled in fine detail. TELEMAC includes horizontal turbulence options for the simulation of very detailed flow patterns, spherical co-ordinates for very large area models, simulation of wetting and drying within the model domain and solution for transcritical flow. TELEMAC-3D can also simulate three-dimensional flow affected by stratification (thermal or saline), wind or wave breaking. Turbulence models available include k-epsilon and mixing length. Two and three dimensional water quality modules are available for use alongside the TELEMAC hydrodynamic modules. Using the water quality modules it is possible to simulate water quality in river, estuarine and coastal regions, in two or three dimensions. Process variables are modelled both in the water column and on the bed so providing a prediction of dissolved, settling and deposited materials. The model is flexible to allow for additional toxic pollutants to be incorporated easily.

Output:
The results from TELEMAC-2D and TELEMAC-3D are often used as input to other modules to study, for example, water quality and sediment transport. Interactions between the following parameters are included within WQ:

- Salinity and Temperature
- Biological Oxygen Demand
- Organic nitrogen
- Ammoniacal nitrogen
- Nitrite; Nitrate
- Dissolved oxygen
- Suspended solids
- Algal carbon and Detrital carbon
- Phosphate
- Silicates
- Hydrogen sulphide
- *E.coli*.

Version and System Requirements:

- TELEMAC-2D: Two-dimensional flows - Saint-Venant equations (including transport of a diluted tracer)
- TELEMAC-3D: Three-dimensional flows - Navier-Stokes equations (including transport of active or passive tracers)

The various modules of the TELEMAC system run on both UNIX and Intel computers under Windows-NT

Application History:

Both WQ-2D and WQ-3D have been applied to major regional and urban pollution studies including environmental impact of reclamations and dredging schemes, strategic water quality planning, outfall design and pollutant dispersion, dredged material disposal, coastal defence design, port and harbour design, navigation and design of shipping channels, wave activity including harbour resonance and failure of dams or dykes.

Availability and Websites:

Contact: HR Wallingford Ltd, Howbery Park, Wallingford,
Oxfordshire, OX10 8BA,
United Kingdom
Tel: +44 (0) 1491 835381
Fax: +44 (0) 1491 832233
Email: info@hrwallingford.co.uk
http://www.hrwallingford.co.uk/software/telemac.html#top

Contact and distributor:

Telemac 2-D	Telemac 3-D
LNH	LNH
J.M.Hervouet	T.Denot
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http://www.telemacsystem.com

TOPMODEL

Description:
TOPMODEL uses a simple conceptualisation of the effect of topography on hydrological fluxes. It calculates catchment outflows and soil surface saturation patterns from precipitation and evaporation time series and from topographic information. A minimum of four effective catchment parameters need to be estimated to characterize the discharge dynamics of the catchment. The parameters are fitted from the discharge predictions. Neither horizontal or vertical soil parameters need to be supplied. However, to estimate water table or soil moisture content from the saturation deficit requires soil information. Surface runoff is computed based on variable saturated areas, subsurface flow using a simple exponential function of water content in the saturated zone. Channel routing and infiltration excess overland flow are considered in the model. The structure of the model with regard to interception and root zone storage compartments is variable, allowing much flexibility to simulated different systems. Time steps should be in the range of an hour to represent surface runoff peaks. The length of the simulation period depends on the availability of precipitation and evapotranspiration input data. The spatial component requires a high quality DEM (digital elevation model) without sinks. A TOPMODEL module has been implemented for the GRASS GIS.

Version and System Requirements:
A Unix-based interface is available through MMS. TOPSIMPL (available in French, English German) has a Windows interface; a Windows version of the model designed primarily for demonstration and teaching purposes is available from Lancaster University.

Assumptions and Limitations:
The model equations are based on the continuity equation, Darcy's Law, and several simplifying assumptions, namely: (1) the hydraulic gradient of subsurface flow is equal to the land-surface slope, and (2) the redistribution of water within the subsurface can be approximated by a series of consecutive steady states. Calibration parameters are relatively few in number and have obvious physical interpretations. TOPMODEL can be applied most accurately to catchments where the assumptions of the model are met, primarily wet catchments that have shallow, homogeneous soils.
One limitation is its dependence on the steady-state groundwater flow equation. A correct estimation of evaporation is critical for model performance. Evaporation is most frequently estimated by using the Penman-Monteith methods. For spruce ecosystems, Haude transpiration was successfully applied.

Availability:
Developer: Lancaster University, UK

Contact: Keith Beven

Centre for Research on Environmental Systems and Statistics

Institute of Environmental and Biological Sciences

Lancaster University, Lancaster LA1 4YQ, UK

Tel:(+44) 1524 593892

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email: K.Beven@Lancaster.ac.uk

Website:

http://www.es.lancs.ac.uk/hfdg/topmodel.html

TRK	The Swedish System

Description:

1. Preparation of areal distribution of different land-use categories and positioning of point sources using GIS;

2. Calculations of concentration and areal losses of diffuse sources (for N from arable land by using the dynamic soil profile model SOILNDB);

3. Calculations of the water balance (by using the distributed dynamic HBV model) and

Data Requirement:

Main model input (sensitive) parameters:

SOILNDB:

Crops

Harvest & crop management

Fertilization and manuring

Soil type (texture) and organic content

Deposition rates & concentration

Meteorological data (air temperature, precipitation, air humidity, insolation, wind speed)

HBV:

Digitalized subbasin boundaries and elevation maps

Land cover

Daily precipitation and temperature from climate stations

Average potential evapotranspiration

Lake rating curve and regulation regime for power damms

Observed time-series of water flow in the river

HBV-N (additional to the HBV-input data):

Soil type and crop distribution of the arable land

Soil leakage concentrations

Lake depths

Atmospheric N-deposition

Point-source N emissions

Rural households and person equivalents of N contribution

Observed time-series of N in the river

TRK-P:

Livestock density

P concentration in topsoil

Runoff

Soil specific area

Assumptions and Limitations:

- Application skills necessary (can also be a strength!)
- Model set-up may be time-consuming
- Simplified process descriptions involves uncertainties
- Internal variables that are unvalidated (involves uncertainties)

Availability:

Main contact:

Helene Ejhed, IVL Svenska Miljöinstitutet AB/ IVL Swedish Environmental Research Institute, Sweden

mailto:helene.ejhed@ivl.se

Alternative contact:

Berit Arheimer, SMHI,

601 76 Norrköping, Sweden

mailto:berit.arheimer@smhi.se

Holger Johnsson, Dep. of Soil Sciences, SLU, Box 7072, 750 07 Uppsala, Sweden

mailto:jonas.olsson@smhi.se

Website:

http://www.euroharp.org/pd/pd/models/TRK-short.html

VISUAL PLUMES Dilution models for effluent discharges

Description:
VISUAL PLUMES is a Windows-based computer application that supersedes the DOS PLUMES. Dilution models for effluent discharges, Third Edition. EPA/600/R-94/086) mixing zone modelling system. VP simulates single and merging submerged aquatic plumes in arbitrarily stratified ambient flow and buoyant surface discharges. Among its new features are graphics, time-series input files, user specified units, a conservative tidal background-pollutant build-up capability, a sensitivity analysis capability, and a multi-stressor pathogen decay model that predicts coliform bacteria mortality based on temperature, salinity, solar insolation, and water column light absorption. VP includes the DKHW model based on UDKHDEN. Initial mixing characteristics of municipal ocean discharges. EPA/600/3-85/073a and b), the surface discharge model PDS (Davis, 1999), the three-dimensional UM3 model based on UM, and the NRFIELD model based on RSB. These models may be run consecutively and compared graphically to help verify their performance. The Brooks equations are retained to simulate far-field behaviour. Finally, DOS PLUMES may be selected as one of the "models," giving full access to its capabilities

Version and System Requirements:
The Visual Plumes model is designed to operate in the Microsoft Windows environment. Properly configured it should run on Windows 95, 98, NT, or 2000 operating systems.

Assumptions and Limitations:
In the usual depth mode, a surface (zero depth, 0) line must be specified in the ambient table. Without this line the ambient array is not set up correctly. One user reported that VP does not run DKHW (and presumably other models) when installed in the E: partition. The same problem occurs when VP is installed as a subdirectory, as for example, to Program Files.

Availability and Website:

U.S. Environmental Protection Agency

Ecosystems Research Division

Center for Exposure Assessment Modeling (CEAM)

960 College Station Road

Athens, Georgia 30605-2700

mailto:ceam@epamail.epa.gov

Software can be downloaded at:

http://www.epa.gov/ceampubl/swater/vplume/index.htm

WASP **Water quality Analysis Simulation Program**

Description:
WASP5 (39) is a generalized framework for modelling contaminant fate and transport in surface waters. WASP5 is the latest of a series of WASP programs (40-43). Based on the flexible compartment modelling approach, WASP can be applied in one, two, or three dimensions. WASP is designed to permit easy substitution of user-written routines into the program structure. Two WASP models are provided with WASP5. The toxics WASP model, TOXI5, combines a kinetic structure adapted from EXAMS2 (44) with the WASP5 transport structure and simple sediment balance algorithms to predict dissolved and sorbed chemical concentrations in the bed and overlying waters. The dissolved oxygen/eutrophication WASP model EUTRO5 combines a kinetic structure adapted from the Potomac Eutrophication Model (45) with the WASP5 transport structure to predict DO and phytoplankton dynamics affected by nutrients and organic material.

Data Requirement:
Simulation and output control, model segmentation, advective and dispersive transport, boundary concentrations, point and diffuse source waste loads, kinetic parameters, constants, time functions, initial concentrations.
WASP5 input and output linkages have been provided to other stand-alone models using formatted ASCII files. Flows and volumes predicted by the link-node hydrodynamic model DYNHYD5 can be read and used by WASP5. Similarly, loading files from PRZM2 and SWMM4 can be reformatted and read by WASP5. DYNHYD5, PRZM2, and SWMM4 are described elsewhere in this paper.

Output:
A menu-driven user interface is provided, along with an interactive graphical post-processor that can create tables and spreadsheet files.

Version and System Requirements:
A Windows 95/98/NT version of WASP, WIN/WASP+, includes a pre-processor, a data processor, and a graphical post-processor (AScI Corporation).

Application History:
Problems that have been studied using the WASP framework include biochemical oxygen demand and dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and organic chemical and heavy metal contamination.

Availability:
Developer: US Environmental Protection Agency (EPA)
Contact:

Model Distribution Coordinator,

Center for Exposure Assessment Modeling,

Environmental Protection Agency,

Athens, Georgia, 706-355-8400,

Email: ceam@epamail.epa.gov

Website:

http://www.epa.gov/ceampubl/swater/wasp/index.htm

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Darcy's law:

Darcy's law describes the flow in an idealised porous media having continuous interconnected pore space. This is flow which is subject to a resistance represented by the hydraulic conductivity (K) of the medium. The governing equations for simulation of flow in porous media having continuously connected pore space are derived mathematically from a combination of Darcy's law and the principle of continuity and allow representation of flow in three dimensions. The derivation is traditionally done by considering the flow through a cube of porous material that is large enough to be representative of the properties of the porous medium and yet is small enough that the change in head within the volume is relatively small i.e. a representative elementary volume (REV). Darcy's law states that

Equation 1: $$Q = KA\ h_L/l$$

where Q is flow rate. K is hydraulic conductivity, A is cross-sectional area, h_L is head loss over the distance l. The continuity (conservation of mass) equation states that

Equation 2: outflow – inflow = change in storage

A general form of the derived equation for non steady-state (transient) flow is

Equation 3: $$\partial/\partial x \left(K_x\ \partial h/\partial x\right) + \partial/\partial y \left(K_y\ \partial h/\partial y\right) + \partial/\partial z \left(K_z\ \partial h/\partial z\right) = S_s\ \partial h/\partial t - R$$

where h is hydraulic head, K_x, K_y and K_z are components of the hydraulic conductivity tensor, S_s is specific storage and R is a general sink/source term that is intrinsically positive and defines the volume of inflow to the system per unit volume of aquifer per unit term. To simulate inflow R = -W, where W is the withdrawal rate. This equation allows for both vertical and horizontal components of flow through the system. A simplified version of this equation is generally used in the simulation of two-dimensional horizontal flow in confined and unconfined aquifers. This used applied where the system consists only of one aquifer of importance to be modelled, confining bed are not explicitly modelled and heads in confining beds are not calculated. Leaky confined aquifers can be simulated using a quasi three- dimensional approach where vertical flow through confining beds is represented by a leakage term which adds or extracts water from the aquifers overlying and underlying the confined leaky aquifer. A general form of this governing equation in two dimensions for transient conditions is

Equation 4: $$\partial/\partial x \left(T_x \, \partial h/\partial x\right) + \partial/\partial y \left(T_y \, \partial h/\partial y\right) = S \, \partial h/\partial t - R + L$$

where h is head, T_x and T_y are components of transmissivity, S is the storage coefficient, R is a sink source term and L a leakance term. When this equation is applied to simulation of two dimensional unconfined flow, the Dupuit assumptions are generally used, specifically, the assumption that the horizontal hydraulic gradient is equal to the slope of the free surface and does not vary with depth. This ensures horizontal flow for the purposes of modelling. The governing equations are extended to non-idealised porous media, including fractured media by using the equivalent porous medium (EPM) approach. Many media have both primary porosity and secondary porosity, in the form of cracks, microcracks, fracture zones, shear zones and weathering fissures. This secondary porosity can exist at a variety of scales, from micro- to macro-scales. The EPM approach assumes that fracture apertures and flow velocities are small enough that Darcy's law applies. The primary and secondary porosities are represented by a continuous porous medium having *equivalent* or effective hydraulic properties. These properties are represented by parameters such that the flow pattern in the EPM is similar to that in the fractured rock. This idea is scale dependant and assumes that for the fractured system there is a representative elemental volume (REV) which is sufficiently large (or small) such that it can be characterised by these effective hydraulic parameter values. Simulation of flow in fractured systems using this method requires definition of effective values for hydraulic conductivity, specific storage and porosity. Working out the scale of area which is required for the REV is difficult but very important. For example, this approach might be appropriate at regional aquifer scale in a waterbody with secondary porosity at either low or high density, since in both cases an appropriate size REV is available. However, while the high fracture density waterbody may also be modelled at local scale, since a relatively small REV is required to define effective parameters, the low density waterbody may not be suitable for modelled at a local scale, since the area to be modelled does not include a sufficiently large REV. The EPM approach is frequently used to represent Irish aquifers, which apart from sand and gravel aquifers are predominantly bedrock media fractured to some degree. In certain karst areas extreme weathering has resulted in the formation of very large fissures, to the point where conduit flow may occur. A system with large fractures can be modelled using the EPM approach where the model domain is sufficiently large to be a REV, and where an estimation of flow at specific points in the fracture system is not required.

Conduit flow:

Conduit flow occurs where individual fractures or fissures in a fractured medium are large enough that flow is not described by Darcy's law. Pollutant Transport Processes are represented conceptually and are described by equations that can be solved in a modelling process. These include *advection*, *dispersion* and *chemical reactions*.

- *Advection* is the process whereby solute is assumed to be transported at the average linear velocity of groundwater (v) which is described by

  Equation 5: $v = -K/n_e \text{ (grad h)}$

  where v is a vector, K is the hydraulic conductivity tensor and n_e is the effective porosity. Advection is the most conservative approach to predicting the speed of movement of pollutant, since it assumes no attenuation of the pollutant occurs.

- *Dispersion* refers to the fact that not all of the contaminant moves at the average linear velocity. Contaminant movement is strongly influenced by the presence of local heterogeneity, which causes deviations from the average linear velocity. Dispersion is described by the first term of the governing equation for solute transport, known as the advection-dispersion equation. Quantification of dispersivity using this equation is very uncertain, complicating unrepresented factors include, the so-called scale effect whereby dispersivity increases with the size of the contaminant plume and the channeling of contaminants along preferential flow paths.

- Owing to difficulty in characterising and representing *chemical reactions*, those reactions represented in solute transport models are limited to adsorption, described by a retardation factor (R_d described by the third term of the governing equation) and hydrolysis and decay, described by a first order rate constant (term four). The governing equation for solute transport, the advection dispersion is

  Equation 6: $\partial/\partial x_i (D_{ij} \partial c/\partial x_j) - \partial/\partial x_i (cv_i) = R_d \partial c/\partial t + \lambda c R_d - C'W^*/n_e$

  where D_{ij} is the dispersion coefficient, c is concentration and C' is a known source concentration, v_i represents the components of the velocity vector, R_d is a retardation factor, λ is a first order rate constant, W* is a source/sink term and n_e is the effective porosity. The first term is the dispersion term, the second represents advection, the third and fourth term represent chemical processes, adsorption and hydrolysis and decay respectively. The fifth term is a sink source term that represents solute mass dissolved in water entering or leaving the model domain. These reactions are adequate only for solving simple contaminant problems and do not take into account any reactions occurring among multiple contaminant species. The transport equations described above apply to miscible fluids, that is fluids which mix and combine readily. Multiphase flow refers to the movement of water and one or more immiscible fluid (or non aqueous phase liquid, NAPL) phases. The governing equations for multiphase flow are different and are formulated in terms of the pressure of each of the phases. Density dependant flow includes salt water intrusion.