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WATER FRAMEWORK DIRECTIVE – An Assessment of Mathematical Modelling in its Implementation in Ireland

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Synthesis Report

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by

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DISCLAIMER

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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.