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WATER QUALITY PREDICTION FOR RIVER BASIN MANAGEMENT

Doctoral Dissertation

Olli Malve

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Helsinki University of Technology
Department of Civil and Environmental Engineering
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Opponent(s)	Prof. Kenneth Reckhow, Duke University, NC, USA
Supervisor	Prof. Pertti Vakkilainen
Instructor	

Abstract

Water quality prediction methods are developed which provide realistic estimates of prediction errors and accordingly increase the efficiency of river basin management and the implementation of EU's Water Framework Directive. The resulting river basin management decisions are based on realistic safety margins for restoration measures and accompanying targeted pollutant load limits.

The realistic error estimates attached to the predictions are based on Bayesian statistical inference and MCMC methods which are able to synthesize two distinct water quality prediction approaches i.e. mechanistic and statistical. What is more, a hierarchical modeling strategy is employed in order to pool information from extensive cross-sectional lake monitoring data and consequently to improve the accuracy and precision of lake specific water quality predictions.

Testing of the methods using extensive hydrological and water quality data from five real–world river basin management cases suggests that Bayesian inference and MCMC methods are no more difficult to implement than classical statistical methods. Even models with large numbers of correlated parameters can be fitted using modern computational methods. Moreover, the hierarchical modeling strategy proves to be efficient for river basin management. Guidelines for adaptive river basin management are also set up based on the experience gained. It is proposed that monitoring, prediction and decision making should be integrated into an efficient management procedure.

Keywords	river basin management, target pollutant load, Bayesian inference, MCMC, hierarchical model	
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Tekijä Olli Malve

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Vedenlaadun ennustaminen vesistöaluiden hoidon suunnittelussa

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Vastaväittäjä(t)	Prof. Kenneth Reckhow, Duke'n yliopisto, NC, USA
Työn valvoja	Prof. Pertti Vakkilainen
Työn ohjaaja	

Tiivistelmä

Tässä työssä kehitetään ja testataan vedenlaadun ennustemenetelmiä, jotka antavat realistisen kuvan ennustevirheistä, auttavat välttämään vesistöalueiden hoitotoimien virhemitoituksen sekä tehostavat EU'n vesipuitedirektiivin toimeenpanoa vastaavasti.

Laskenta perustuu Bayeslaisen päättelyyn ja MCMC -menetelmään, jotka mahdollistavat mekanistisen vedenlaatumallin ennustevirheen realistisen estimoinnin. Lisäksi sovelletaan hierarkista mallintamisstrategiaa järvikohtaiseen vedenlaadun ennustamiseen laajan suomalaisen järviseuranta-aineiston perusteella. Valittu strategia pienentää ennustevirheitä ja parantaa ennusteiden tarkkuutta.

Menetelmiä testataan Lappajärven, Kymijoen, Tuusulanjärven, Säkylän Pyhäjärven sekä yli kahden tuhannen, Suomen ympäristökeskuksen seurantaverkossa olevan järven hoitotoimien tavoitteen asettelussa. Testit osoittavat, että Bayes-päättelyn ja MCMC-menetelmän ja klassisten tilastomatemaattisten menetelmien laskennallinen toteutus on yhtä helppoa. Jopa suuren määrän korreloituneita parametrejä sisältävä vedenlaatumalli saadaan sovitettua havaintoaineistoon. Myös hierarkinen mallintamisstrategia on tehokas väline vesistökohtaisten vedenlaatuennusteiden tekemisessä ja vesistöalueiden hoidon suunnittelussa. Lopussa annetaan suosituksia vesistöseurannan, vedenlaadun ennustamisen sekä vesistöjen hoidon yhdistämisestä tässä työssä kehitettyjen laskentamenetelmien avulla jatkuvasti tarkentuvaksi, adaptiiviseksi hoitoprosessiksi.

Asiasanat vesistöaluiden hoito, tavoite kuormitus, Bayes päättely, MCMC, hierarkinen malli

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Preface

The statistical inference methods adopted during the preparation of this thesis opened up new vistas of endeavour in scientific discovery and learning and revealed their usefulness for the identification and interpretation of constraints on river basin management and for the specification of limits for sustainable water and land use.

Professor Pertti Vakkilainen, the supervisor of this work and head of Water Resources Laboratory at Helsinki University of Technology, and Olli Varis, are warmly acknowledged for their guidance and encouragement.

The Finnish Environment Institute (SYKE) is thanked for the opportunity to carry out this study as a part of my work there and to test the methods in real–world river basin management projects and for access to the institute's valuable databases. The supportive and stimulating research environment provided by Juha Kämäri, Seppo Rekolainen and Matti Verta is particularly acknowledged.

The writer's co-authors and colleagues at SYKE and elsewhere are warmly thanked for their efforts, knowledge, skills and sharing of data during the progress of the work: Teija Kirkkala, Mauri Pekkarinen, Olli-Pekka Pietiläinen, Simo Salo, Jouko Sarvala, Matti Verta, Kristiina Vuorio and Jarmo Vääriskoski who were particularly involved in the acquisition of the chemical and biological water quality data and John Forsius, Heikki Haario, Timo Huttula, Marko Laine, Kari Lehtinen, Simo Salo and Song Qian, who were concerned with the computational implementation of water quality predictions.

The author was privileged to visit the Water Quality Laboratory of the Nicholas School of the Environment and Earth Sciences at DUKE University in 2004 – 2005. It was a once in a lifetime opportunity to acquire new viewpoints to statistical

decision making in river basin management. Professor Kenneth Reckhow, George Arhonditsis, Chi-Feng, Jacqui Franklin, Andrew Gronewold, Melissa Kenney, Conrad Lamon and Song Qian are warmly thanked for their friendship and new ideas. Conrad Lamon is particularly acknowledged for reviewing this summary.

Juhani Kettunen and Elja Arjas, the preliminary examiners of this thesis, are warmly thanked for their precise and constructive comments, which improved the summary to a decisive extend, and also Malcolm Hicks, who reviewed the English language of it.

The work was supported in part by the Centre for International Mobility, the EU FP5 research project BMW (Benchmark Models for the Water Framework Directive, Contract EVK1-CT-2001-00093), Maa- ja vesitekniikan tuki ry, the Academy of Finland's research project MaDaMe (BIAS sub project; Development of Bayesian methods with applications in geophysical and environmental research), the EU FP6 research project REBECCA (Relationships between the ecological and chemical status of surface waters, Contract SSPI-CT-2003-502158) and the Sven Hallin Foundation.

Finally, I'm overwhelmed with gratitude to my beloved wife, Anne, our dear daughters, Sara, Kaisla and Kirsi and my parents, Heimo and Raili Malve for their constant love and to God who paved the way for this thesis.

Helsinki, April 2007

Olli Malve

Contents

List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.

I Malve, O., Huttula, T. and Lehtinen, K. 1991. Modelling of Eutrophication and Oxygen Depletion in the Lake Lappajärvi. In: Wrobel, L., Brebbia, C.(Eds.), Water Pollution: Modelling, Measuring and Prediction. Computational Mechanics Publications, pp. 111–124.

II Malve, O., Salo, S., Verta, M. and Forsius, J. 2003. Modelling the transport of PCDD/F compounds in a contaminated river and possible influence of restoration dredging on calculated fluxes. Environmental Science & Technology, 37(15), pp. 3413–3421. DOI: 10.1021/es0260723

III Malve, O., Laine, M. and Haario, H. 2005. Estimation of winter respiration rates and prediction of oxygen regime in a lake using Bayesian inference. Ecological Modelling, 182(2), pp. 183–197. DOI:10.1016/j.ecolmodel.2004.07.020

IV Malve, O., Laine, M., Haario, H., Kirkkala, T. and Sarvala, J. 2006. Bayesian modelling of algae mass occurrences – using adaptive MCMC methods with a lake water quality model. Environmental Modelling and Software, 22(7), pp. 966–977. DOI:10.1016/j.envsoft.2006.06.016.

V Malve, O. and Qian, S. 2006. Estimating nutrients and chlorophyll a relationships in Finnish Lakes. Environmental Science & Technology, 40(24), pp. 7848–7853. DOI: 10.1021/es061359b.

Author's contribution

Table 1: Account of author contribution. Names are in alphabetic order. Abbreviations of authors: FJ (Forsius, J.), HH (Haario, H.), HT (Huttula, T.), KT (Kirkkala, T.), LM (Laine, M.), LK (Lehtinen, K.), MO (Malve, O.), SS (Salo, S.), SJ (Sarvala, J.), VM (Verta, M.) and QS (Qian, S.)

Contribution	*Paper*				
	I	*II*	*III*	*IV*	*V*
1. Data and mass balances	HT LK MO	MO SS VM	MO	KT LM MO SJ	MO
2. Currents and sediments	HT LK MO	MO SS VM	MO	-	-
3. Computational implementation	HT LK MO	FJ MO SS	HH LM MO	HH LM MO SJ	MO QS
4. Fitting and validation	HT LK MO	MO SS	HH LM MO	LM MO	MO QS
5. Water quality prediction	HT LK MO	MO SS	HH LM MO	LM MO	MO QS
6. Interpretation of results	HT LK MO	MO SS VM	HH LM MO	HH LM MO SJ	MO QS

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1 Introduction

1.1 Background

The availability of clean water and the good ecological status of surface waters have been endangered by increasing loads of nutrients and chemicals. In 2000-2003 water quality was satisfactory or worse in 20 – 27 per cent of the Finnish lake, coastal and sea area and in twice that proportion of the river area (50 %). To improve and protect water quality in watercourses, the Finnish government passed the Water Act on 19 May 1961 and legislation for the assessment of environmental impacts on 10 June 1994. The new set of national Water Protection Policy Outlines extending to 2015 was approved on 23 November 2006, under which diffuse nutrient loading from agriculture should be reduced by a one third by 2015 and loading from fish farming and waste water treatment plants must be further reduced. In particular, nitrogen removal from municipal waste water must be improved to 70 % in densely populated areas with more than 10,000 inhabitants.

The general goals of the Water Framework Directive, introduced by the European Union on 22 December 2000, are to achieve a ”good status” in all water bodies by 2015 and to protect the aquatic ecology, unique valuable habitats, drinking water resources and bathing water with reasonable costs. Planning and implementation of water management will be organized on a river basin basis in order to ensure that local factors and the need for water protection measures are taken into account efficiently. Ecological and chemical protection is required everywhere, but other forms of protection will apply only within specific zones.

An act on the organization of river basin management planning was adopted in Finland in 2004, and the drafting of plans was started by the regional working groups. The plans will be complete by 2009 and will be updated every six years.

For these purposes, Finland has been divided into five river basin districts, two international river basin districts (the Tornio River and the Teno – Näätämö – Paatsjoki district) and to a separate river district covering the autonomous province of the Åland Islands.

The targeting of the required pollutant load reductions and the finding of technical solutions for their implementation are the challenging key ingredients of the river basin planning, and all our existing science, technology, mathematics and practical experience in this field will be needed to achieve compliance with the water quality standards with regard to chemical substances and ecological status. Hydrological and biogeochemical cycling, in particular, and the resource conditions for the assembly of the plankton community must be considered comprehensively. Until quite recently the theoretical foundation for ecology was empirical rather than theoretical, ranging from deterministic to stochastic approaches, and hence there is no equivalent comprehensive biological foundation analogous to Newtonian mechanics or hydrodynamics that can be employed for the control of eutrophication and pollution in lakes and rivers. In addition, the determination, calibration and validation of prediction models is hampered by the overwhelming number of factors affecting the composition and activity of plankton assemblages and by the limited experimental and observational resources available. Hence the translation of scientific theories, specific observations on river basin and mathematical approaches into forms which are useful for river basin planning is difficult.

Prediction models are nevertheless considered useful for river basin management and are used to predict the behaviour of water quality with respect to changes in pollutant loads and hydrological conditions. They are therefore used to evaluate target pollutant loads and management actions which will achieve compliance with water quality standards. The target pollutant loads are then used to set up regulatory rules and to plan waste water treatment plants, agricultural practices and general land use.

Simple empirical water quality models are based on statistical methods, which makes quantitative learning and prediction efficient (Manly, 2001; Berthouex and Brown, 2002). Early attempts were made in the 1970'sto estimate statistical relationships in data from a large sample of lakes (Vollenweider, 1976; Vollenweider and Kerkes, 1980; Reckhow and Chapra, 1983), and more complex mechanistic models (Jørgensen, 1980; Chapra and Reckhow, 1983; Orlob, 1983; Chapra, 1997) were structured in the 1970's according to the causal understanding and mathematical descriptions of processes prevailing at that time, sometimes accompanied by least-squares parameter estimates, approximate first order error analysis, Monte Carlo analysis or Kalman filtering (Scavia, 1980). The error term in a model was usually neglected in the context of prediction (NRC, 2001). The lack of proper error estimates was compensated for by a comprehensive mathematical description of the process. Thus, the development of mechanistic models for water quality and hydrodynamics were seen to be interrelated (Streeter, 1958; Chow, 1959; Graf, 1971; Cunge et al., 1980; Dyer, 1986; van Rijn, 1989). Water quality management in Finland has often been supported by a combination of empirical and mechanistic models (Kinnunen et al., 1982; Frisk, 1989; Sarkkula, 1991; Varis, 1991; Kettunen, 1993; Nyroos, 1994; Huttula, 1994; Kokkonen, 1997; Rankinen, 2006).

1.2 Research problem

The EU Water Framework Directive urges member states to quantify numerically the present and near-future maximum loads (i.e. target pollutant loads) to be permitted for pollutants, from point and non-point sources and from background sources, so that they will meet water quality standards with an adequate margin of safety (MOS). Due to the probabilistic and random nature of water quality parameters, a small MOS might result in non-attainment of the water quality goal, while a large MOS can be inefficient and costly (NRC, 2001). Therefore the MOS should account for the errors in the data and the model. Ideally, MOS represents the

joint probability of possible errors in the estimated target load, load estimates and transcendence of the water quality standards (NRC, 2001). The problem is how to estimate model parameters and error variances of predictions realistically and determine how errors in these and in the inputs propagate through the model and result in error in the estimated target pollutant load.

Another problem is that approximate error estimation methods involving complex mechanistic water quality models and small-sized water quality samples are likely to result in unrealistic (Ascher and Overholt, 1983; NRC, 2001) and overly optimistic error estimates (Omlin and Reichert, 1999). This in turn will bias the MOS of the target pollutant loads and reduce the efficiency of river basin management. (Figure 1.1).

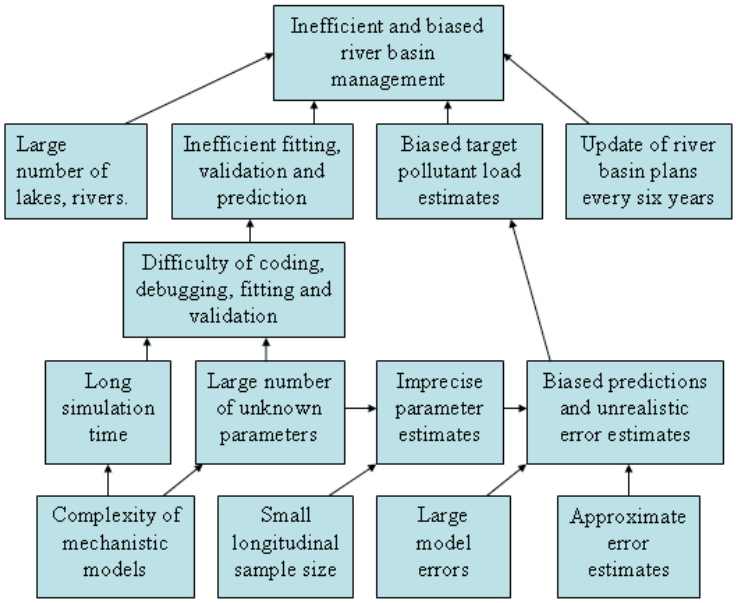

Figure 1.1: Outline of the problems involved in water quality prediction and their implications for river basin planning and management.

The coding, debugging, fitting and validation of complex mechanistic water quality

models is difficult due to the long simulation time and the large number of unknown parameters, making water quality prediction and river basin management less efficient and more costly than is necessary for effective decision making (NRC, 2001). Moreover, twenty per cent of the Finnish lake area is in a satisfactory or worse condition, which means that the number of lakes requiring pollutant load control amounts to hundreds and the updating of river basin plans every six years using complex water quality models will not be efficient or even feasible.

1.3 Objectives

The general objective of this thesis were to make the updating of water quality predictions, the accompanying error estimates and river basin plans every six years as efficiently and realistically as possible (Figure 1.2). It was aimed at using Bayesian inference, Markov chain Monte Carlo methods (MCMC), hierarchical models (HM) and model simplification. Bayesian inference and MCMC methods were to be used for synthesizing mechanistic modelling and statistical inference and facilitating realistic error estimation and the efficient updating of predictions in the light of the continuously accumulating monitoring data. A hierarchical modelling strategy (Gelman and Hill, 2006) was used to improve the accuracy and precision of lake specific the predictions.

The practical objectives were computational implementation of the methods, the derivation of relevant water quality data, application of these methods to real-world river basin management cases and the setting up of guidelines for applications to river basin management.

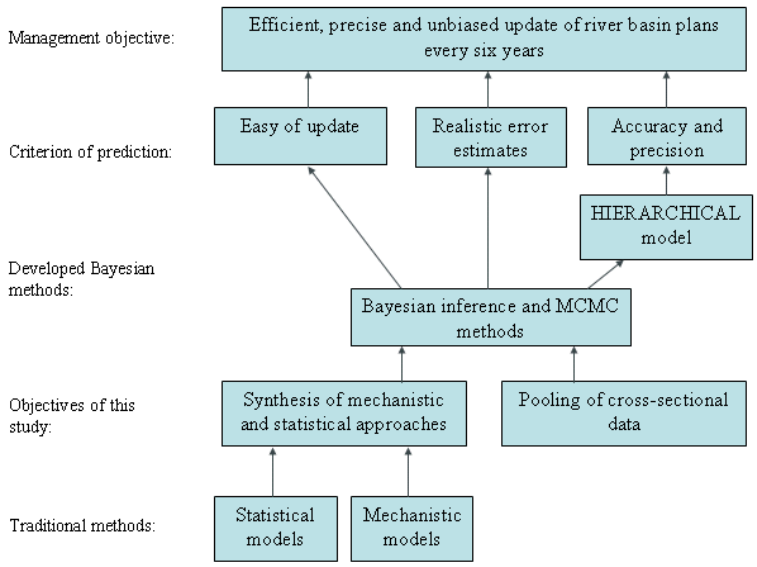

Figure 1.2: General objectives of river basin management and the methods developed in this study.

1.4 Scope of the research

A complex mechanistic lake and a river model was first developed to facilitate the prediction of water quality in connection with river basin management. A full statistical error analysis of sub water quality models was then accomplished using Bayesian inference and MCMC methods. The error analysis of some extremely complicated models was postponed because the converge of MCMC sampling algorithms is slow if a model includes a large number of correlated parameters. Instead, the moderately simple lake respiration and phytoplankton sub models were analysed initially. This clearly revealed the advantages and limitations of Bayesian inference and MCMC methods and motivated the use of adaptive sampling algorithms and simple linear models. Prior distributions, if informative, were obtained from the scientific literature or from experimental and observational data. Expert elicitation techniques were not used here.

To make the water quality prediction and management in large river basins with small observational sample sizes more tractable, hierarchical models were also applied. These were based on causal relationships among a small number of descriptors.

The mechanistic water quality models constructed for Lake Lappajärvi and the River Kymi linked river basin management measures directly to water quality responses, whereas the water quality sub models which were fitted using Bayesian inference and MCMC methods were limited in this sense. Later on, the model of a entire water body were fitted using MCMC methods.

1.5 Research methods

The mechanistic lake models used here described vertical mixing, temperature stratification, respiration, sedimentation, leaching of nutrients and phytoplankton growth. The river model calculated the longitudinal dispersion of suspended solids and contaminated sediments. The models were formulated with partial and ordinary differential equations and integrated by numerical methods.

A hierarchical linear regression model (HLRM) (Gelman and Hill, 2006) was used to predict chlorophyll a in Finnish lakes. Hierarchical linear modelling (HLM), also known as multi-level analysis, is a more advanced form of multiple linear regression. Multilevel analysis allows the variance in outcome variables to be analysed at multiple hierarchical levels, whereas in multiple linear regression all effects are modelled as occurring at a single level. Thus HLM is appropriate for use with nested data. In river basin management, data from lakes can be nested within lake types and ecoregions.

The errors in the mechanistic and hierarchical models (f in equations 1.1) are related to errors in the measurement of the x variables (ϕ^2), in the model (σ^2) and in the

model parameters (σ_θ^2) (Box and Tiao, 1973; Clark, 2006). These were estimated using Bayesian inference and MCMC methods, which facilitate statistical learning and the updating of water quality predictions and river basin plans.

$$\begin{aligned} & y_j = f(x_j;\theta) + \epsilon_j \\ & \theta \sim p(\mu_\theta, \sigma_\theta^2) \qquad \text{'error in parameters'} \\ & \epsilon_j \sim N(0,\sigma^2) \qquad \text{'model error'} \\ & x_j^{(obs)} \sim p(x_j, \phi^2) \quad \text{'error in } x\text{'} \end{aligned} \tag{1.1}$$

1.6 Contribution

Bayesian inference methods and Markov chain Monte Carlo (MCMC) methods were used here to change the paradigm of water quality prediction and river basin management decision making from deterministic to statistical. Mechanistic river and lake models for the evaluation of target phosphorus loading and restoration dredging were developed and applied in papers I and II (Table 1.1), and the best features of the mechanistic and statistical prediction methods, i.e. the deterministic simulation and the full statistical error analysis, were synthesized in papers III and IV. This enabled the mechanistic water quality predictions to be better accommodated into river basin management. The slow convergence of the MCMC chains in the case of marked parameter correlation was speeded up by means of adaptive Metropolis Hastings methods. The accuracy and precision of the lake-specific chlorophyll a predictions based on extensive cross–sectional monitoring data of Finnish lakes were enhanced using a hierarchical linear regression model.

The main results of the five original papers listed at the beginning of this publication will be summarized below. The papers are referred to in the text by their Roman numerals. First, the case data and the objectives of river basin management cases

will be analysed, and then the selected water quality prediction methods and their capabilities for meeting the objectives of river basin management will be evaluated. Finally, guidelines for water quality prediction in adaptive river basin management will be proposed.

Table 1.1: Contribution of the papers to water quality prediction and river basin management.

Mechanistic modeling —>	*Bayesian inference*
Paper I:	
-*Probe lake model*: prediction of vertical convection and diffusion of heat, dynamics of dissolved oxygen, total phosphorus and chlorophyll a -assessment of target phosphorus load	
Paper II:	
-*One dimensional sediment model*: prediction of longitudinal transport of contaminated sediments -setting up of a criterion for restoration dredging	
Paper III:	
-*Respiration model*: prediction of dissolved oxygen regime in a lake	-*MCMC method*: Unbiased error estimates, pooling of cross-sectional information -design and real time control of oxygenation devices
Paper IV:	
-*Lake phytoplankton model*: prediction of algal blooms	-*MCMC method*: same as in Paper III -target nutrient and zooplankton biomass concentrations
Paper V:	
	-*MCMC method*: same as in Paper III -*Hierarchical linear chlorophyll a model*: nutrient to chlorophyll a relationship, enhanced pooling of cross-sectional information -target nutrient concentrations

2 Observational data

The observational data used here originated from three intensively studied Finnish lakes (I, III and IV), a river (I) and 2289 sparsely monitored Finnish lakes (V). Lake Lappajärvi (I), Lake Tuusulanjärvi (III) and Lake Pyhäjärvi in Säkylä (IV) are locally important for fishing and recreation, but their use is hindered by eutrophication, which impairs also their ecological status. This led the Finnish Environment Institute (SYKE), the regional environment centres, the universities, local authorities, private enterprises and water protection associations to contribute to the sampling and management of these lakes. The Southeast Finland Environment Centre and SYKE had sampled the sediments and water of the River Kymi and planned restoration dredging of contaminated sediments. The water and sediment samples representing the lakes and the river had not been randomized, except for the zooplankton sample from Lake Pyhäjärvi, which was randomized according to a stratified design. In general, the samples were concentrated spatially in the middle of the lake or of the river cross-section, and the water samples from the River Kymi were from points both upstream and downstream of the area of main interest. The sampling time was confined to the open water period, except for the sampling of dissolved oxygen in Lake Tuusulanjärvi, which took place when the lake was covered by ice.

2.1 Lake Lappajärvi

Lake Lappajärvi is a shallow lake in the western part of Finland (Figure 2.1) that is agriculturally loaded, mesotrophic and has occasional algal blooms. The bottom sediment at the two main depths (1 km^2) becomes anoxic during the summer and winter stratification periods and 5 mg $m^{-2}d^{-1}$ phosphorus is released into the water body. The theoretical retention time is 2.8 years. Phosphorus is the main limiting

nutrient for phytoplankton growth. Loading in the lake is 0.38 gP $m^{-2}a^{-1}$ and its sedimentation coefficient R is about 0.8. The mean phosphorus concentration in the lake is 23.8 μg l^{-1} and the mean fresh biomass concentration of planktonic algae is 2.7 mg l^{-1}.

The lake water level, outflow, vertical temperature profile, currents, ice cover and snow cover were observed in the years 1987 - 1989. Daily meteorological data were collected at Kauhava Airport 30 km west of the lake.

Water quality in five inflows and the flow between the two sub-basins of the lake were investigated intensively (2-12 times a month) in May 1. 1988 - April 30. 1989, together with sedimentation rate experiments and flow measurements (Figure 2.1).

2.2 River Kymi

The River Kymi is the fourth largest river in Finland. It has been polluted by effluents from pulp mills and the chemicals industry and through some tributaries and diffuse non-point sources. Loading has been reduced considerably, but the remains of past emissions still exist in the river sediments. The area studied here is a 130-km stretch of the river with branches between Lake Pyhäjärvi (in Jaala) and the Gulf of Finland (Figure 2.2). There are 11 power plants and 6 stretches of rapids on this reach of the river. The upper part of the river strech is 50 m above sea level and the mean slope of the river bed is small (0.0006). The drainage area of the River Kymi is 37 200 km^2 (lake percentage 18%), with only 3% (1 100 km^2) running directly into the stretch of the river. Thus 97 % of the water in the river at this stage comes from upstream sources. The mean discharge at the downstream end of the river is 330 m^3 s^{-1}.

The river bed in this area consists mainly of transport and erosion sites, which con-

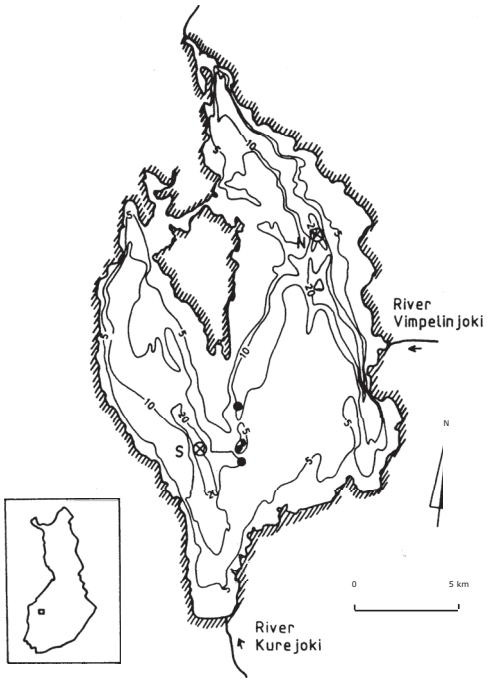

Figure 2.1: Map of Lake Lappajärvi. Observation points= Water samples, = Current meter, = Thermistor chain.

tain non-cohesive soil or solid clay and silt. At wider points in the river there are sedimentation pools, which are the main traps for PCDD/F compounds. Contaminated organic particulate materials accumulated earlier in the main sedimentation pool at Kuusankoski, and this sediment is nowadays decomposing slowly, eroding and migrating downstream. The transported sediment with highest settling velocity has accumulated in the downstream sedimentation pools, whereas the smaller particles have migrated to the estuarine and the marine area. Due to hydrological regulation at the power plants, the sediments have not been exposed to high floods and discharges have not increased. Construction projects and changes in river regulation imply a risk of the mobilization of PCDD/F compounds in the future.

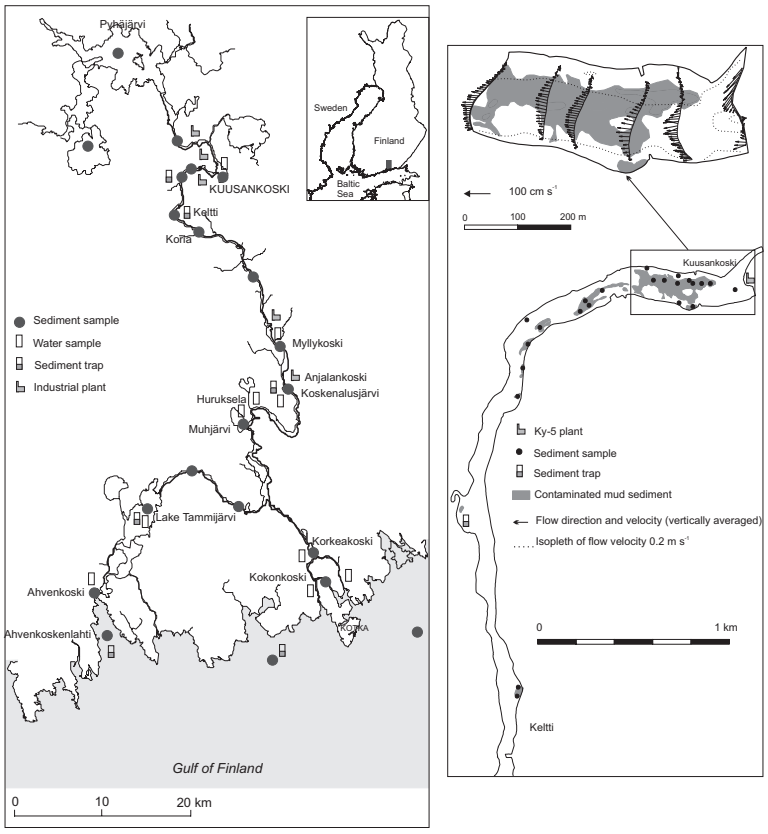

Figure 2.2: Map of the River Kymi.

The hydrological and hydraulic data (water level and discharge) needed to perform the sediment transport calculations were observed at least daily or even more frequently at the power plants and stretches of rapids. Suspended solids concentrations upstream and along the relevant stretch of the river were observed frequently enough for calibration. The observations of direct runoff and corresponding concentration of suspended solids do not cover the whole catchment, however. Monthly values for suspended solids from industrial effluent point loading were collected from sewage treatment plants, and non-point loading was estimated from the continuous runoff data and weekly water quality samples from two small representative catchments

(30 and 178 km^2) in the drainage area (1 100 km^2)). The transported sediment was sampled with sediment traps at six locations and PCDD/F concentrations in the sediment were analysed. No direct measurements of historical PCDD/F loading from Kuusankoski are available, but the amount of historical PCDD/F loading from the Ky-5 plant and from eroding sediments in Kuusankoski and its variation were estimated from a bottom sediment sample originating from the bay of Ahvenkoskenlahti at the mouth of the river (Figures 2.2).

2.3 Lake Tuusulanjärvi

Lake Tuusulanjärvi is a shallow, hypereutrophic lake located just north of Helsinki in southern Finland, lat. 60° 26' long. 25° 03' (Fig. 2.3). Having previously been mesotrophic, it became hypereutrophic in the 1960s due to sewage discharge. The winter dissolved oxygen regime was in a critical condition in the early 1970s, but improved slightly in 1973, when winter aeration was introduced. The situation was further improved by reductions in nutrient loading. Sewage discharge was diverted in 1979 and summer aeration started in 1980. The hypereutrophic condition remained, however, and blooms of blue-green algae have occurred every summer since the loading reduction (50% in phosphorus loading) in 1979. The phosphorus load from agriculture (4500 kg a^{-1} = 0.75 g m^{-2} a^{-1}) still exceeds the lake's tolerance level, which is why a reduction in the phosphorus content of the water body by intervening in both external and internal phosphorus loading has been required.

The lake water was sampled at two-metre vertical intervals at the deepest point in the lake (max. depth 10 m by the Uusimaa Regional Environment Centre and the local water protection board (Keski-Uudenmaan vesiensuojelun kuntayhtymä) during the period 1968–2003. Samples were collected 2–7 times each winter for the analysis of dissolved oxygen concentration and temperature by standard methods. Vertical averages and standard deviations were calculated. Dissolved oxygen con-

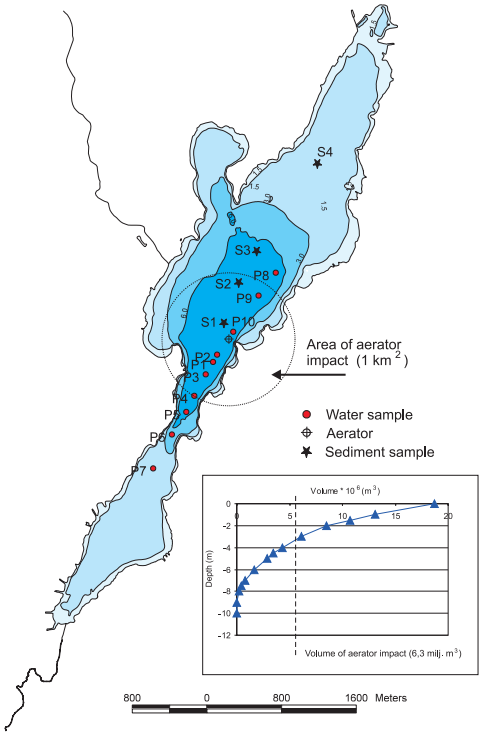

Figure 2.3: Map of Lake Tuusulanjärvi.

centrations were also measured in situ at nine stations in March 2001 to determine the area of aerator impact.

Winter net oxygen consumption in the lake in the early 1970s was estimated to be 200 000 kg on average. The flux of the pumped dissolved oxygen as estimated by the aerator consultants (100 tn on average) shows a high yearly variation due to technical problems and fluctuations in the duration of the ice-cover. This leaves a significant uncertainty concerning the estimated dissolved oxygen fluxes, which affects the lake respiration estimates. The value describing the prior distribution was calculated from information available in technical reports.

Table 2.1: Hydrology and morphology of Lake Tuusulanjärvi (Anonymous, 1984).

Surface area	6.0	km^2
Volume	$19 * 10^6$	m^3
Maximum depth	10	m
Average depth	3.2	m
Length (max)	7.5	km
Theoretical water residence time	250	d
Area of drainage basin	92	km^2
Percentage of lakes in the drainage basin	8.4	%

Table 2.2: Characteristics of the catchment of Lake Pyhäjärvi.

Total area (inclusive of lake's surface)	615 km^2
River Yläneenjoki	234 km^2
River Pyhäjoki	77.5 km^2
Remaining area (small sub-basins)	149.5 km^2

2.4 Lake Pyhäjärvi in Säkylä

Lake Pyhäjärvi is a shallow, mesotrophic, agriculturally loaded lake (Fig. 2.4) in which algal blooms increased in the early 1990's. All the major cyanobacterial blooms in 1992–1999 were dominated by *Anabaena flos-aquae* (Lyngb.) Breb., while *Anabaena planctonica* Brunnt., *Anabaena curva* Hill, *Cyanodictyon reticulatum* (Lemm.) Geitl., and *Aphanothece clathrata* W. & G.S. West became dominant in 1999.

Monitoring of the water chemistry and hydrology of Lake Pyhäjärvi started in the

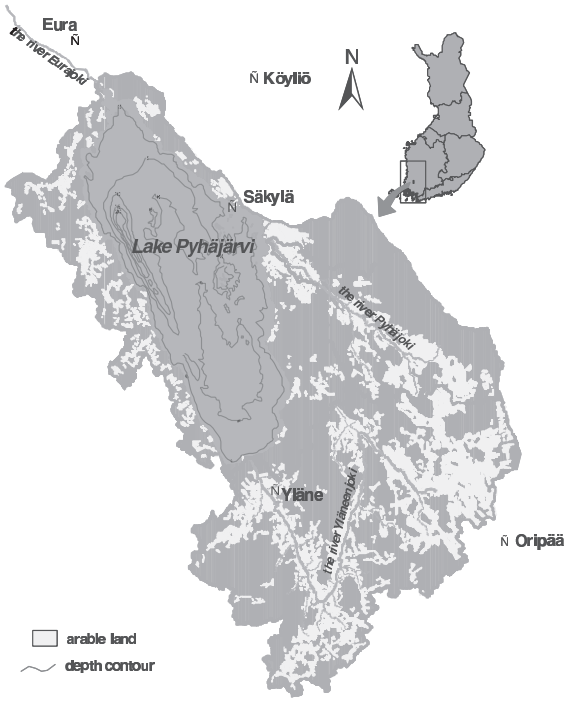

Figure 2.4: Map of Lake Pyhäjärvi.

1960s, and intensified monitoring of nutrient concentrations was started by the Water Protection Association of SW Finland in 1980 and continued from 1993 onwards by the Southwest Finland Regional Environment Centre. Vertical profiles were taken at the deepest point in the lake 6–8 times during the open water period in 1980–1991 and at two-week intervals in recent years. Due to the openness and shallowness of the lake, there is no extended stratification during the summer. Nutrient and plankton concentrations are vertically and horizontally homogeneous most of the time (Sarvala and Jumppanen, 1988). Phytoplankton was sampled together with nutrients and counted at the Department of Biology, University of Turku (Sarvala et al., 2000). Zooplankton was sampled at approximately weekly intervals from the surface to the bottom at ten locations selected with a stratified random design

Table 2.3: Characteristics of Lake Pyhäjärvi.

Surface area	155 km^2
Volume	849 million m^3
Mean depth	5.4 m
Maximum depth	26 m
Coastline	110 km
Water residence time	3–5 year

(Sarvala et al., 2000). Crustacean zooplankton was enumerated at the Department of Biology, University of Turku. Eight years of observations collected between 1992 to 2000 were used for this study. Our data set contains the biomass concentrations of Diatomophyceae, Chrysophyceae, nitrogen-fixing Cyanobacteria and minor groups of phytoplankton summed together, total phosphorus concentration (TP), total nitrogen concentration (TN), water temperature (T), global irradiance (I), the biomass concentrations of grazing zooplankton (Z) and outflow rates (Q).

Sarvala et al. (1998) have shown that year-to-year variations in chlorophyll a and phosphorus concentrations in Lake Pyhäjärvi are associated with changes in the total biomass of planktivorous fish, good fish stocks being accompanied by depressed zooplankton biomass and high chlorophyll a levels. One-third of the total variation in chlorophyll a is attributed to changes in zooplankton biomass and another third to the changes in phosphorus concentrations.

2.5 Finnish lakes

National water quality monitoring in Finnish lakes started in 1965, after the passing of the Water Act in 1962, when information was required on the status, quality and

quantity of Finnish water resources, and how their status relates to and responds to pressures on the environment. The sampling strategy and analytical methods have been described by Niemi et al. (2001). A geomorphological typology of Finnish lakes is under construction to aid in the classification of their ecological status. According to a preliminary topology they may be divided into the nine types according to their surface area, depth and water colour (Table 2.4).

Table 2.4: Preliminary geomorphological typology of Finnish lakes as specified by the Finnish Environment Institute (SA=Surface Area, D=Depth).

Lake Type	*Name*	*Characteristics*
I	Large, non-humic lakes	SA $>$ 4,000 Ha, color $<$ 30
II	Large, humic lakes	SA $>$ 4,000 Ha, color $>$ 30
III	Medium and small, non-humic lakes	SA: 50 - 4,000 Ha, color $<$ 30
IV	Medium, humic deep lakes	SA: 500 - 4,000 Ha, color: 30–90, D $>$ 3 m
V	Small, humic, deep lakes	SA: 50 - 500 Ha, color: 30–90, D $>$ 3 m
VI	Deep, highly humic lakes	Color $>$ 90, D $>$ 3 m
VII	Shallow, non-humic lakes	Color $<$ 30, D $<$ 3
VIII	Shallow, humic lakes	Color: 30-90, D $<$ 3 m
IX	Shallow, highly humic lakes	Color $>$ 90, D $<$ 3 m

19,248 observations of total phosphorus, total nitrogen and Chlorophyll a (Chla) in 2,289 Finnish lakes in July and August from 1988 to 2004 were used in this study. About 42% of the observations were from July and 58% from August. On the other hand, observations were unevenly distributed between the years, lake types (Table 2.5) and individual lakes. 900 lakes out of the 2,289 lakes were represented by only one observation, but the average number of observations was eight (s.d. 26) per lake. One lake had 441 observations, and there were 12 lakes that had more than 150.

Table 2.5: Number of observations (N) within the lake types.

Type	*N*	*Type*	*N*	*Type*	*N*
1	485	4	3,949	7	391
2	6,536	5	1,080	8	2,729
3	388	6	1,326	9	2,544

2.6 Analysis of the case data

The observational data were used to establish a basis for river basin water quality prediction and management. Ideally, a water body should be sampled according to statistical design methods in order to minimize the error variances in the model, but in the present case the data were collected according to intuitively selected rules and the model for prediction and decision making was selected later.

Certain important features of the data (Table 2.6) were analysed retrospectively (Table 2.6) to reveal the adequacy of the data set for water quality prediction and river basin management. One of the most important features in this respect was the sample size because a small sample size may reduce the precision of a prediction, and thus the overall efficiency of river basin management (Figure 1.1). The case studies involved extensive sample sizes. The predictions were also affected, however, by the orientation of the sampling design. The data for the case studies were mainly longitudinal, except for the monitoring data on the Finnish lakes, which were abundant in a cross-sectional direction, i.e. covering numerous lakes. On the other hand, the majority of the lakes were observed only a few times, so that the lake specific samples were small and unbalanced, reducing the precision of the lake-specific predictions. A small sediment respiration experiment conducted in Lake Tuusulanjärvi and the parameter ranges obtained from the scientific literature for the River Kymi, Tuusulanjärvi and Pyhäjärvi models can be regarded as small

extensions in a cross-sectional direction.

Table 2.6: Analysis of case study data.

Classifier	Lappajärvi	Kymijoki	Tuusulanjärvi	Pyhäjärvi	Finnish lakes
Sample size	Extensive	Extensive	Extensive	Extensive	Extensive
Orientation of sampling design	Longitudinal	Longitudinal	Longitudinal	Longitudinal	Cross-sectional
Hierarchical structure	Single level	Single level	Single level	Single level	Hierarchical
Scientific discipline	Hydrology Chemistry Biology	Hydrology Chemistry Biology	Hydrology Chemistry Biology	Hydrology Chemistry Biology	Chemistry
Sampling design	Intuitive	Intuitive	Intuitive	Intuitive	Intuitive
Treatment method	Observational	Observational	Observational	Observational	Observational

If data are hierarchically structured, i.e. they include multilevel or nested clusters within which correlations occur, cross-sectional information can be pooled to make longitudinal predictions more precise by means of hierarchical or multilevel models. The Finnish lake data were hierarchically structured (with the levels: all lakes, type of lake, lake), and this feature was utilized in modeling phase. The rest of the data did not have a hierarchical structure.

The scientific discipline of data handling may involve notable variation in sample size, in that there is a common tendency for the numbers of biological observations to be smaller than those of chemical or hydrological observations. This was also the

case in the present case studies.

The careful selection of sampling design and treatment method, which are of great importance for water quality prediction, was left out of the data acquisition process in the majority of the cases studied here. Sampling was not randomized, and experimental design methods were not employed other than in the case of Lake Pyhäjärvi where zooplankton was sampled using a stratified random design.

3 Objectives of river basin management

3.1 General objectives

The general objectives of water quality management in river basin planning and decision making are sustainable use and management of the waters and their good ecological status (Figure 3.1). The first things to be decided are the water quality standards and the acceptable probability of these being exceeded. Water quality standards include numerical values for threshold values separating attainment from non-attainment of the management objectives with respect to the given variables. The water quality predictions can then be used to infer target pollutant loads which will achieve compliance with the water quality standards (Figure 3.2) and to generate a set of feasible management actions in the planning phase with a view to the cost and benefit analysis in the decision phase.

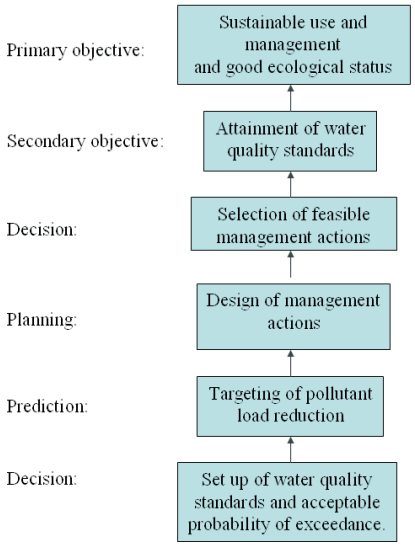

Figure 3.1: General objectives of water quality management in river basin planning.

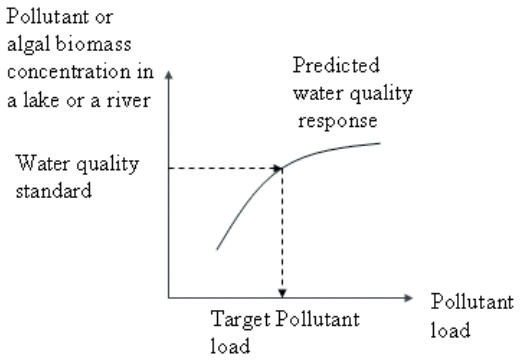

Figure 3.2: Inference of target pollutant loading using predicted water quality response i.e. pollutant or algal biomass concentration in a lake or a river. Water quality standards include numerical values for threshold values separating attainment from non-attainment of the management objectives with respect to pollutant concentration.

3.2 Objectives in case studies

3.3 Lake Lappajärvi

The objective of the management of Lake Lappajärvi was to limit chlorophyll a to below 10 μg l^{-1} (Figure 3.3). The target phosphorus load that complied with this criterion was selected from a number of phosphorus load scenarios and simulated chlorophyll a concentrations. The simulations were based on the hydrological, meteorological and phosphorus loading data for the one-year period April 1 1988 - March 31 1989. Responses were calculated at four loading levels: 1. present 0.35 gP m^{-2} a^{-1} 2. Fast obtainable reduction (14.8 % reduction) 0.30 gP m^{-2} a^{-1} 3. Desirable level (32.7 %reduction) 0.23 gP m^{-2} a^{-1} 4. Best available protection measures (44.9 % reduction) 0.19 gP m^{-2} a^{-1}.

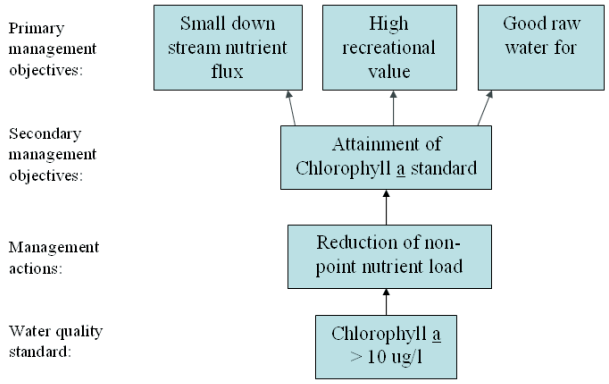

Figure 3.3: Management objectives, actions and water quality standard for Lake Lappajärvi.

3.4 River Kymi

The objective of management in the case of the River Kymi was to dredge or permanently immobilize sediments which were contaminated by dioxin compounds at Kuusankoski (Figure 3.4). Dredging, if implemented, would have to be performed in such a way that the migration of dioxin was minimized. Canalization of the river, dredging of the most seriously contaminated sediments and a number of smaller construction projects on the river constituted notable risks of further pollutant migration, and the migration of contaminated sediments and the exposure of the river and its adjacent marine and human populations to PCDD/F compounds were predicted in order to assess these risks.

3.5 Lake Tuusulanjärvi

The objective of the management of Lake Tuusulanjärvi was to lower the trophic status of the lake, which is the primary reason for oxygen depletion in its water, fish deaths and the excessive internal phosphorus loading (Figure 3.5). The means

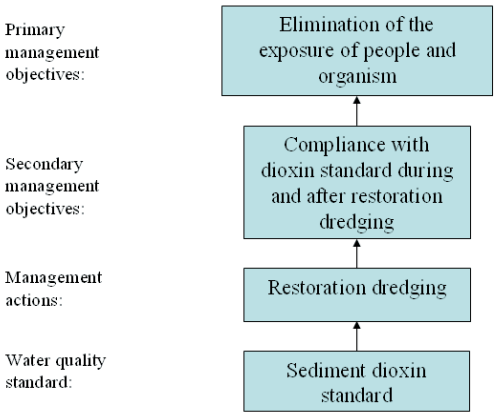

Figure 3.4: Management objectives, actions and water quality standards for the River Kymi.

chosen for this have been artificial oxygenation, reduction of external nutrient loads, dilution of the lake water with nutrient-poor water from a neighboring water body, and control over fishing. The effect of artificial oxygenation on the dissolved oxygen regime and the real-time control of oxygenation devices were studied here.

3.6 Lake Pyhäjärvi

The objectives of management in Lake Pyhäjärvi were to improve its ecological status, recreational value and fish catches (Figure 3.6). This was to be done by reducing the external nutrient load and controlling fishing. Farmers have been participating in water protection projects initiated by the Southwest Finland Regional Environment Centre (SFREC) in 1991 and coordinated by the Pyhäjärvi Protection Fund since 1995 (Ventelä et al., 2001). The necessary reductions in nutrients and the optimal fishing management strategy will remain under continuous scrutiny all the time the decrease in the occurrence of algal blooms and in nutrient concentrations take place only slowly.

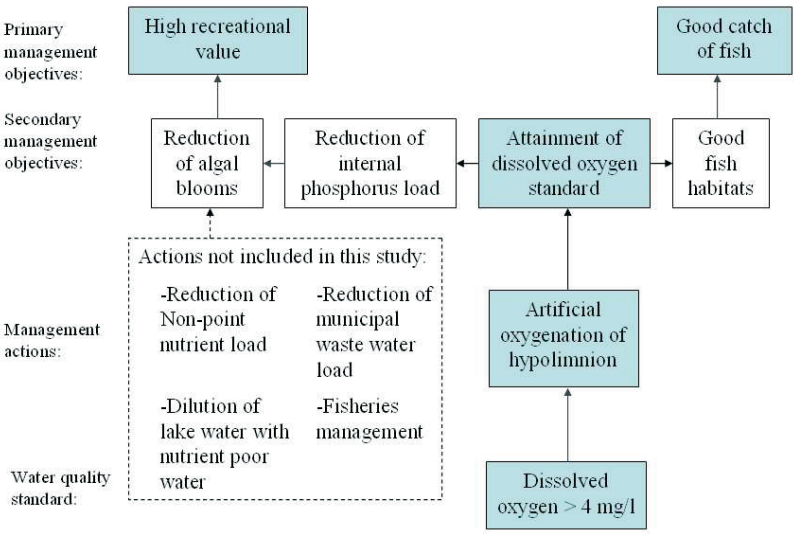

Figure 3.5: Management objectives, actions and water quality standard for Lake Tuusulanjärvi.

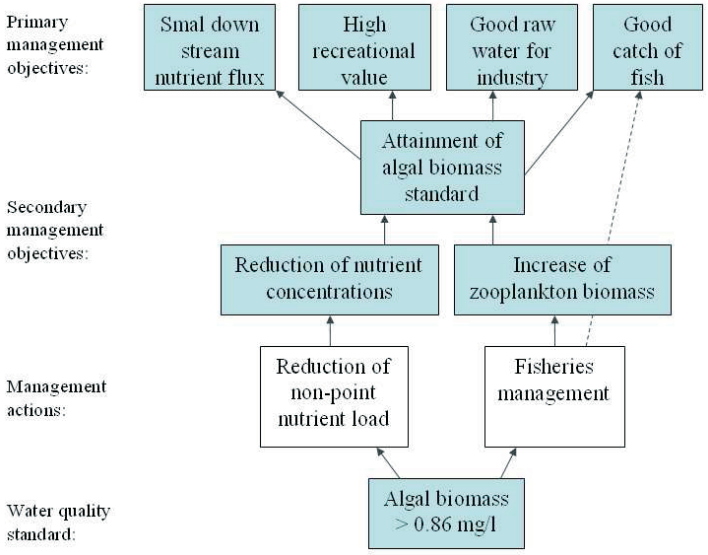

Figure 3.6: Management objectives, actions and water quality standards for Lake Pyhäjärvi in Säkylä.

3.7 Finnish lakes

The objective of the management of the Finnish lakes was to restore them to a good ecological status (Figure 3.7). This involved reducing their nutrient load to a level that meets the chlorophyll a standard, a proxy for a phytoplankton standard.

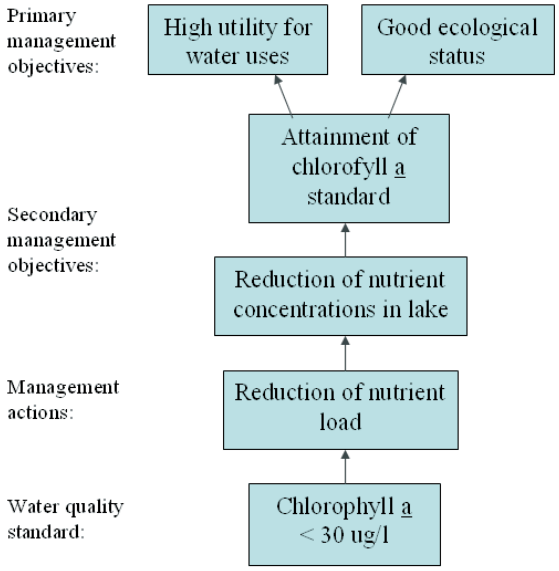

Figure 3.7: Management objectives, actions and water quality standards in the Finnish lakes.

4 Evaluation of prediction methods

4.1 General objectives

The main objectives of prediction in river basin planning are to acquire and analyse all the information necessary and to provide accurate and precise predictions of the expected water quality outcomes of planned management actions (Table 4.1). Since management decisions are usually made under conditions entailing considerable predictive uncertainties, realistic estimates of the possible error contained in predictions are needed. In addition, the adjustment of river basin plans every six years calls for continuous monitoring of water quality, analysis of management success and correction of failures. Ideally, this should be achieved by continuous updating of the parameters and predictive distributions. On the other hand, the precision of lake-specific (longitudinal) predictions will be low if the sample size is small. Higher precision can be achieved most efficiently using estimation methods which are able to pool cross-sectional information in order to make longitudinal inferences. The accomplishment of the above objectives are expected to promote efficient river basin planning and management.

Table 4.1: Criteria for predictions in river basin planning.

Accuracy and precision
Realistic error estimates
Ease of updating predictions
Coverage of large geographical areas
Pooling of cross-sectional data to longitudinal inference
Efficiency

4.2 Classification of prediction methods

Water quality prediction methods can be classified by reference to several attributes, the most important among which are the modelling approach, the structure of the model and the scientific discipline concerned (Figure 4.1). According to this classification, the prediction approach can be either mechanistic, statistical or Bayesian, where a mechanistic approach relies on comprehensive process description using numerical integration of partial or ordinary differential equations (Jørgensen, 1980; Chapra and Reckhow, 1983; Orlob, 1983; Chapra, 1997), while statistical prediction is based on classical statistical point estimation, which is somewhat approximate if applied to mechanistic models (Omlin and Reichert, 1999). In contrast, a Bayesian approach can combine mechanistic process description and observational data resulting in a posterior predictive distribution, which is useful in river basin management (Box and Tiao, 1973; Clark, 2006).

Models are classified here in terms of their structure and that of the data used as either hierarchical or composed of a "single" level (Gelman and Hill, 2006). Classical "single" level estimates may be useless if fitted to a lake with a small sample size and misleading, in that they ignore variation between lakes and lake types if fitted to composite data representing different lake types. A hierarchical model allows the estimation of lake and lake type-level effects and can achieve a compromise between noisy and oversimplified classical estimates. A hierarchical linear regression model was used here together with a geomorphological typology of Finnish lakes to estimate the nutrient effect on chlorophyll a in lakes of varying sample sizes. For example, a linear or generalized linear model in which probability models are assigned to the regression coefficients can be considered as a hierarchical model. This second level has parameters of its own, which are also estimated from the data.

A water quality prediction method can be classified in terms of scientific discipline as either hydrological, chemical or biological. Hydrological predictions are often

based on numerical integration of complicated continuity equations of mass, energy and momentum, while chemical and biological reaction kinetics are normally approximated using ordinary differential equations or steady state linear regression models.

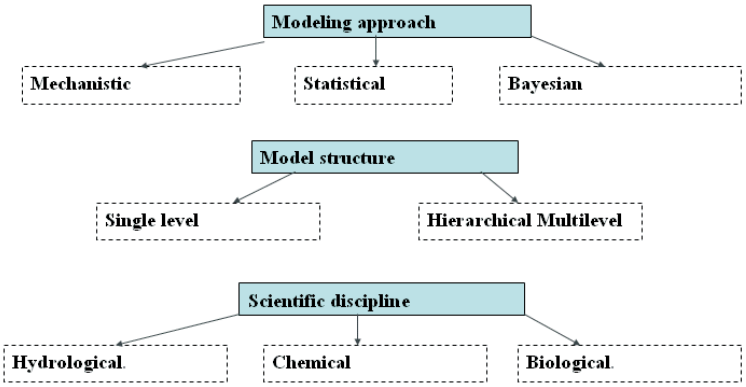

Figure 4.1: Classifiers of prediction methods.

4.3 Bayesian inference using MCMC methods

Bayesian inference

A Bayesian approach facilitates continuous updating of parameters, error variances and predictions as new information accumulates (Figure 4.2). Bayesian methods do this formally as

$$\text{posterior} \propto \text{likelihood} \times \text{prior} \tag{4.1}$$

The likelihood ($p(y|\theta)$) and prior density $p(\theta)$ for a parameter enable calculation of the posterior density $p(\theta|y)$, the distribution of which for an unknown parameter θ

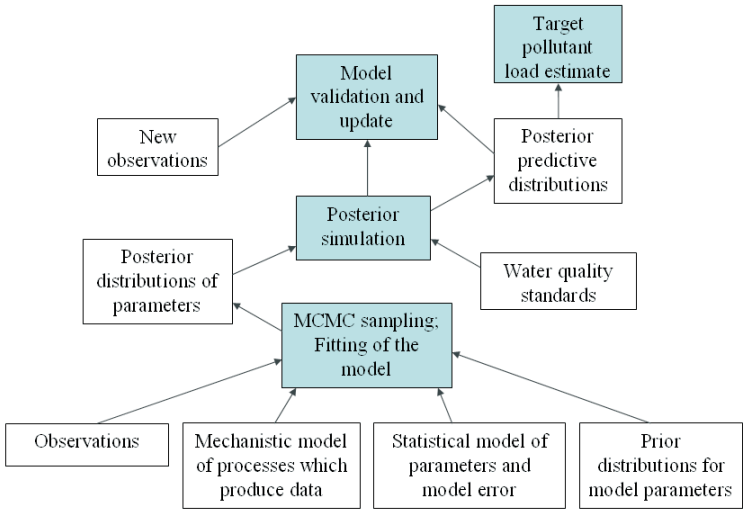

Figure 4.2: Elements of Bayesian posterior predictive inference in target pollutant load estimation.

is formulated as:

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} = \frac{p(y|\theta)p(\theta)}{\int_{-\infty}^{+\infty} p(y|\theta)p(\theta)d\theta} \tag{4.2}$$

The posterior density consists of the product of the likelihood and the prior distribution divided by the normalization constant. The integral in the normalization constant $\int_{-\infty}^{+\infty} p(y|\theta)p(\theta)d\theta$ for a complex model is hard to calculate analytically, but fortunately integration is not needed if Monte Carlo methods are used for posterior simulation. This involves drawing repeated random samples of the parameter or parameter vector. Several methods exist for posterior simulation and prediction, among which the Markov chain Monte Carlo (MCMC) method allows simulation of multivariate distributions and is usually implemented as a random walk through the parameter space. During the 'burn-in' period the Monte Carlo averages converge to the target distribution, after which samples of parameters are used to

estimate the posterior distribution. Non-standard distributions are sampled here using Metropolis-Hastings (Hastings, 1970; Haario et al., 1999, 2001, 2003, 2004; Clark, 2006) and Gibbs sampling (Gelman et al., 2005; Spiegelhalter et al., 1996, 2002; Clark, 2006).

Prior distributions

To fit the models to Bayesian methods, a prior distribution for the parameters needs to be specified. Since prior independence of the parameters was assumed, only a marginal density for each component of the parameter vector was assigned here.

The strongest form of prior assumption is that a parameter is a fixed constant, e.g. as obtained from literature. Alternatively, a 'fixed' constant may be treated as a parameter with a narrow prior distribution. If no prior value is known or if we want the posterior value to depend solely on the observed data, a flat "non-informative" prior assumption is preferred, perhaps with a positivity constraint, as with many of the parameters in the present cases. Nevertheless, every new parameter increases the dimension of the vector to be sampled and increases the computational burden. Mainly Gaussian prior distributions with possible upper and lower limits for the values (e.g. positivity constraints) are used in the present work.

Model error

Since the models described the system on a non-transformed scale, they had to be transformed accordingly for the fitting procedure. The observational error was modelled as a Gaussian random variable. The errors in the lake respiration and chlorophyll a models were additive with respect to the modelled concentration, and the error term ϵ_i in the phytoplankton model was additive with respect to the square

root of the modelled concentrations:

$$\sqrt{y_i(t)} = \sqrt{\mu(x_i;\theta)} + \epsilon_i \tag{4.3}$$

where ϵ_i is the error term. The error term of the model contains all the unexplained factors, and may include several sources of errors other than pure observational error. The error term is assumed to follow a Gaussian distribution with unknown variance. We used a standard non-informative conjugate prior variance defined by an inverse gamma distribution.

MCMC sampling

The Bayesian inferences regarding the respiration, phytoplankton and chlorophyll a parameters in the model were implemented using MCMC sampling methods. Instead of a single fit to the data, statistical distributions were determined for the model parameters. In practice, the process involved four steps: 1. Formulation of prior probability distributions for unknown model parameters. 2. Statistical analysis of measurement errors. 3. Specification of likelihood function. 4. MCMC (Markov chain Monte Carlo) sampling of the posterior probability distributions of the parameters and predictions.

The Bayesian approach has been shown to be a powerful way of quantifying the uncertainties in the whole modelling procedure (Adams, 1998; Annan, 2001; Borsuk, 2001; Borsuk et al., 2001; Harmon and Challenor, 1996; Omlin and Reichert, 1999; Reckhow, 2002; Qian et al., 2002). The MCMC computations and adaptive MCMC strategies used here are demonstrated and described in Haario et al. (2003). MCMC is popular in computational statistics at the moment (Gelman et al., 2005) and can be applied to a wide variety of modelling problems (Gamerman, 1997).

Although recent advances in MCMC computing and increasing CPU resources have made larger problems tractable (Haario et al., 2001), computational problems still arise on account of correlations between parameters. The limited availability of observational data and the structure of non-linear modelling equations may cause correlation between parameters, which can be reduced through better design of the experiments and reparametrization of the model. In situ monitoring does not favour orthogonal observational design for generating completely uncorrelated observations of independent variables, however, and adaptive MCMC methods have been developed as a remedy (Haario et al., 2001). Adaptive methods make the procedure statistically efficient and reduce the need for laborious hand tuning of the algorithm. In fact, they adapts the proposal distributions for the generation of new samples according to the Adaptive Metropolis algorithm (AM) instead of using a fixed proposal distribution. In addition, a number of different scales for the proposal distribution were used, employing the Delayed Rejection (DR) method (Haario et al., 2001, 2003, 2004).

The number of iterations that the Monte Carlo averages need to converge to the true posterior distribution is called the burn-in period. Samples obtained after the burn-in were saved for statistical inference of the posterior distribution. To ensure convergence and to estimate the lake respiration and phytoplankton dynamics, several runs were carried out sequentially, each sequence starting from the values of the previous chain, and convergence was diagnosed visually from 1d and 2d plots of the chains. In contrast, the length of the burn-in period for the hierarchical regression model, multiple MCMC chains of different length were run and $\hat{R}$ statistics (Gelman and Rubin, 1992) were calculated for each chain. If $\hat{R} \approx 1$ the burn-in period was deemed adequate.

Posterior simulation

Where Bayesian inference and MCMC methods were used for model fitting, the water quality responses to planned pollutant load reductions and management actions were predicted using posterior simulation methods. Predictions were calculated repeatedly with sampled parameter values and error variances from their posterior distribution and with relevant environmental control variables derived from their observed distributions. The simulated predictive distributions revealed prediction errors realistically and rationalized river basin management accordingly.

4.4 Model validation

Prediction with mechanistic models was mainly based on a theoretical understanding of the underlying mechanism and the consequent causal relationships. Runs with data located outside the range of variation of the calibration data were used to confirm the model and to reveal structural errors and limitations in it.

Validation in an empirical modelling approach is clearly related to the scientific learning process (Kettunen, 1993; NRC, 2001; Brun et al., 2001; Omlin and Reichert, 1999; Reichert and Vanrolleghem, 2001; Clark, 2006), where a tentative model suggests an experiment or observational data gathering process and an appropriate analysis of the data can lead to a new experimental or observational design (Box and Tiao, 1973). The alternation between the model and experiment is carried out by means of experimental design and data analysis. The efficiency of the underlying statistical learning process depends on the appropriateness and power of the design and analysis methods employed. In Bayesian analysis, a prior distribution is combined with the data to calculate the posterior distribution, from which inferences regarding the parameters are to be made. The postulated probability model is never

expected to be entirely true, but is chosen in the light of the available knowledge and constructed with the simplest possible structure. It must therefore be tested at each step in the investigation. Residual quantities are calculated and sensitivity to prior distributions and model structure are tested to criticize the probability model and to suggest modifications.

Comprehensive validation of mechanistic models is a luxury that is seldom achieved in water quality management, due to limitations caused by sparse data and the complicated model structure. Scientific learning using statistical analysis methods involves a continuous iterative approach in which management decisions are conditional on the validity of the tentative model and the available information. River basin management decisions thus have to be modified alongside this iterative learning process and model criticism.

The validation of the mechanistic water quality model for Lake Lappajärvi was hampered by the small observational water quality sample size, which meant that the data could not be separated out into calibration and validation sets. By contrast, one-year data on dioxin concentrations in settling suspended solids were available for validation of the transport model for the River Kymi. The respiration model for Lake Tuusulanjärvi and the chlorophyll a model for the Finnish lakes were not validated, either, but the phytoplankton model for Lake Pyhäjärvi was validated with data from 5 additional years. The residual normality of the respiration, phytoplankton and chlorophyll a models was investigated through a graphical display of the predictive distributions and observations. Sensitivities to prior distributions and model structure were not studied.

To facilitate comparison of the hierarchical linear model with non-hierarchical dummy variable models, we calculated the deviance information criterion (DIC), a Bayesian measure of model complexity and fit (Spiegelhalter et al., 2002). DIC is the sum of the posterior mean deviance $\overline{D(\theta)}$, a Bayesian measure of fit or "adequacy", and a

complexity measure p_D (effective number of parameters), which corresponds to the trace of the product of Fisher's information and the posterior covariance.

4.5 Analysis of case predictions

4.5.1 Lake Lappajärvi

Prediction method

A water quality model was constructed to link phosphorus loading and hydrological conditions to phytoplankton growth and oxygen deficit in Lake Lappajärvi (Figure 4.3). The driving variables included wind, cloudiness, air temperature, humidity, water outflow and the phosphorus loads from point and non-point sources.

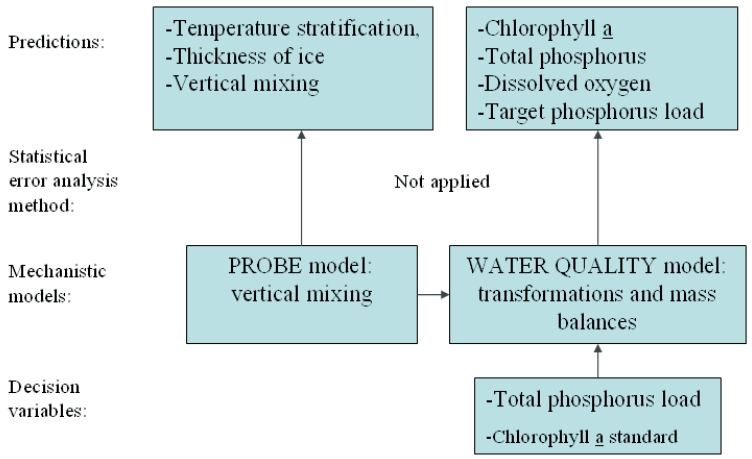

Figure 4.3: Decision variables, prediction methods and predictions for water quality management in Lake Lappajärvi.

Vertical mixing and temperature distribution were simulated by means of a one-dimensional, horizontally integrated, k-e turbulence model, PROBE (Svensson, 1986;

Svensson et al., 2002). It was assumed that the lake was horizontally homogeneous and that gravitational effects obeyed the Boussinesq approximation. A complete description of the model and the numerical scheme are given by Svensson (Svensson, 1977, 1978; Svensson et al., 2002).

The ice increment was calculated using a degree-day method, while the melting formulation took the decreasing ice thickness to be a linear function of air temperature. The model distinguished between ice increment or melting on the basis of the direction of the net surface heat flux.

The water quality model coupled with the PROBE model simulates vertical mixing and chemical and biological transformations of total phosphorus, dissolved oxygen and chlorophyll a (a proxy for phytoplankton biomass). The transformations were biological oxygen demand, phytoplankton growth and respiration, respiration in the bottom sediment, growth, respiration and settling of chlorophyll a, external phosphorus load, sedimentation and internal phosphorus load under anaerobic conditions.

Model calibration and prediction

The simulated temperatures and ice thicknesses agreed well with the values observed in 1987 - 1988, but the modelled temperature stratification in late August was ten days longer than observed and a mean error of 1.5 days arose in the ice duration. Of the water quality model parameters, the BOD decay rate, sediment oxygen demand, net sedimentation of phosphorus, phosphorus release from the sediment under anaerobic conditions, algal growth, algal respiration and rate of chlorophyll a sedimentation were calibrated with one year of observed data (May 15, 1988 - April 30, 1989). Parameters were fitted to predict average chlorophyll a, dissolved oxygen and total phosphorus concentrations. Calibration was carried out graphically without

mathematical parameter optimization or error analysis methods. The model over predicted chlorophyll a to a moderate extent. The mean squared error (MSE) was 29.6, the sum of squares (SS) was 355 and the root mean square error (RMSE) was 5.4.

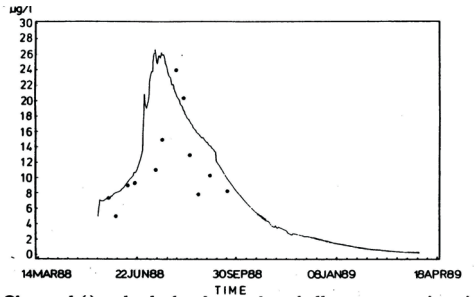

Figure 4.4: Observed and simulated chlorophyll a concentrations [μg l^{-1}] in Lake Lappajärvi, May 15, 1988 - April 30, 1989.

The study of the effects of the reduction in non-point source phosphorus loading on chlorophyll a was based on the hydrological, meteorological and phosphorus loading data collected from April 1, 1988 to March 31, 1989. Since chlorophyll a as predicted with scenario number 4 (the best available protection measures, 44 % reduction) (Fig. 4.5) was below the standard (10 μg l^{-1}), the respective load (0.19 gPm^{-2} a^{-1}) was selected as a target nutrient load for lake management. As the model error and parameter and predictive distributions were not estimated, and the long-term variation in control variables was not measured or used in the simulation, the computed effects ignored natural variation and predictive uncertainty. Hence, it is not possible to calculate an explicit margin of safety for the target phosphorus load estimates.

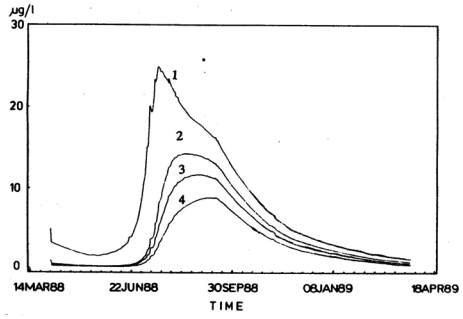

Figure 4.5: Calculated chlorophyll a concentration [μg l^{-1}] with loading levels: 1.Present (in April1. 1988 - March 31. 1989) 0.35 gP m^{-2} a^{-1} 2. Fast obtainable load reduction(14.8 % reduction) 0.30 gP m^{-2} a^{-1} 3. Desirable loading level (32.7 %reduction) 0.23 gP $m^{-2}a^{-1}$ 4. Best available protection measures (44.9 % reduction) 0.19 gP m^{-2} a^{-1}.

4.5.2 River Kymi

Prediction method

Flow velocity, water level and the transport of contaminated sediments and PCDD/F compounds along the 130 km stretch of the River Kymi were calculated using a one-dimensional (1-D) river model (Figure 4.6). The model was also used to calculate time series and longitudinal profiles for suspended solids and PCDD/F concentrations in the river water and bottom sediment. The resulting model was then applied for the evaluation of the impact of dredging on the transport of PCDD/F compounds downstream in the river and into the Gulf of Finland.

In the 1-D unsteady river flow model, the full de Saint Venant equations were solved numerically with a double-sweep finite difference method in which Verwey's variant of the Preissmann implicit discretization scheme was used (Cunge et al., 1980). The resistance term was calculated using the Manning approach, with the Manning number taken as an empirical constant (Cunge et al., 1980). The 1-D sediment

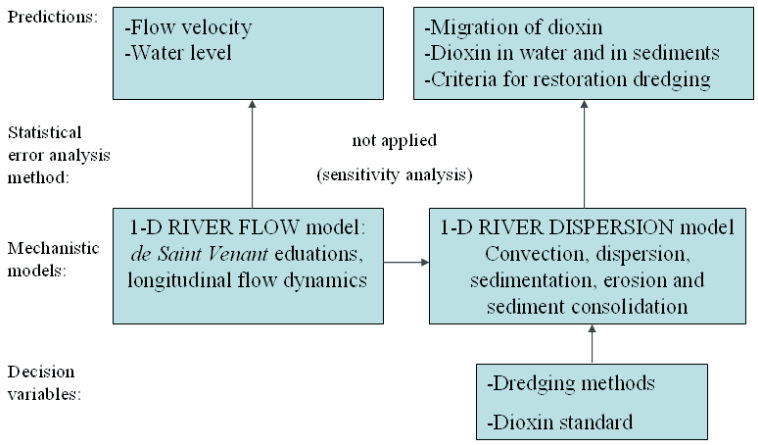

Figure 4.6: Decision variables, prediction methods and predictions for water quality management in the River Kymi.

and contaminant transport model was used to calculate the convection, dispersion, sedimentation and erosion of suspended solids and PCDD/F with unsteady flow (Cunge et al., 1980), and the model was linked to the flow model. The sedimentation rate of suspended solids in the river water and rate of erosion of the bottom sediments were calculated as functions of shear stress. The bottom sediment was divided into 4 layers with differing consolidation times, and the values for these constants were selected according to the sediment properties analysed. PCDD/F compounds were assumed to migrate adsorbed to particulate matter.

Model calibration and prediction

A large amount of information was collected and assimilated into the 1-D hydraulic river model. The settling velocity of suspended solids w_s was calibrated with observations from 1980 to 1996, and the calculated PCDD/F concentrations in the river and the PCDD/F concentrations analyzed in the sediment trap samples in 1997 were compared (Figure 4.7) in order to validate the model. The model approx-

imated the main features of PCDD/F transport successfully but somewhat over predicted PCDD/F concentrations in the sediments at the downstream end of the river.

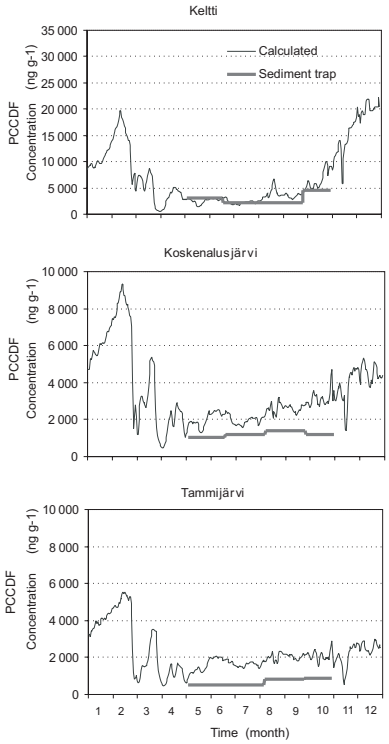

Figure 4.7: Model verification. Calculated PCDD/F concentrations in suspended solids in the river water, and concentrations observed in sediment traps in 1997.

The effects of the dredging and removal of contaminated sediments at Kuusankoski over the period 2000-2020 were examined based on two responses: the immediate increase in suspended solids and PCDD/F concentrations in the water caused by dredging in 2005 and the subsequent decrease. It was assumed that the most contaminated sediments (140 000 m^3) between Kuusankoski and Keltti (Figure 2.2) would be removed by dredging during a half-year period. Based on earlier experience, from 1% to 10% of the sediment removed was expected to be resuspended in

the river water. The PCDD/F concentration in the dredged and resuspended bottom sediment was 40 400 ng g^{-1} (140 ng I-TEQ g^{-1}). In this case PCDD/F loading would be about 300 kg. The model predicted that the simulated restoration dredging would cause a sudden increase in PCDD/F concentrations in the river unless implemented carefully (Figure 4.8), but that concentrations would soon decrease to a significantly lower level than before dredging. The estimated sensitivity of the model to sediment parameters within the specified ranges did not indicate high risk of the spreading of PCDD/F compounds.

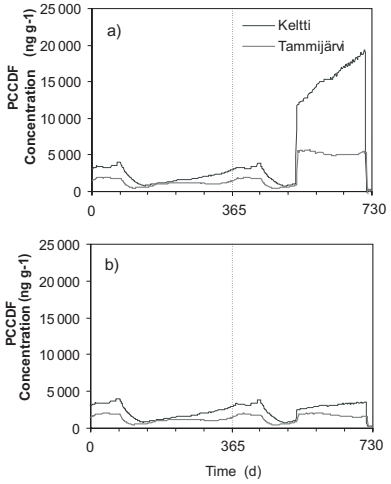

Figure 4.8: Calculated PCDD/F concentrations [ng g^{-1}] in suspended solids in the upper (Keltti) and lower (Tammijärvi) river stretches of the River Kymi before, during (days 534–713) and after dredging, on the assumption that 10 % (a) or 1% (b) of the dredged sediment would be resuspended in the river water.

4.5.3 Lake Tuusulanjärvi

Prediction method

In standard lake aeration planning techniques, the average winter respiration rate in the lake is typically estimated with linear regression, where the y variable is the dissolved oxygen content of the water body [mg m^{-2}] and the x variable the time after the beginning of the ice-cover period [d]. The slope of the regression line represents the respiration rate [mg m^{-2} d^{-1}] (Lorenzen and Fast, 1977). In this study, a dynamic ordinary differential equation was formulated (Figure 4.9) that consisted of respiration and the oxygen flux of the aerator. The temperature dependence of the respiration was calculated according to the Arrhenius formulation (Bowie et al., 1985). The dissolved oxygen concentration was the average vertical concentration in the area of aerator impact (1 km^2, Fig. 2.3). Due to the fact that the biological oxygen demand (BOD) was below the detection limit in winter periods, it was not included in the model. A similar formulation has been used for modelling estuarine and coastal oxygen dynamics (Borsuk, 2001; Borsuk et al., 2001).

The respiration model for Lake Tuusulanjärvi included 31 respiration rate parameters, one for each winter period, and 31 initial dissolved oxygen concentrations. The temperature dependence constant θ was assumed to be independent of time, and thus added only one parameter. The error in the x variables approach for the dissolved oxygen feed term introduced five more parameters. Together with the unknown observation error σ^2, the total number of parameters totalled 69.

Prior distributions

To fit the respiration models using Bayesian inference and MCMC methods, a prior distribution was specified for the parameters.

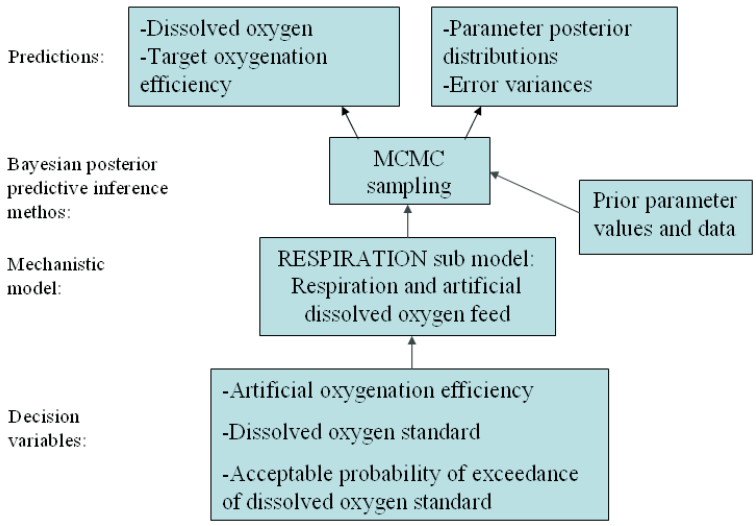

Figure 4.9: Decision variables, prediction methods and predictions for water quality management in Lake Tuusulanjärvi.

Non-informative prior distributions were used to explore the posterior distributions for the total respiration rate constants (one for each winter period) without any prior constraints (other than positivity). The proper prior distribution for the temperature dependence parameter θ was acquired from a laboratory experiment (Lehtoranta and Malve, 2001). The distribution suggested by the experiment was Gaussian $\mathrm{N}(1.45, 0.4)$. A non-informative conjugate prior distribution was used for the unknown variance σ^2 in the observation error ϵ.

The term $\frac{\text{feed}}{\text{vol}}$ in the model corresponds to the amount of fresh oxygen feed dissolved in the lake water. The feed estimated by the manufacturer and the volume of aerator impact are also subject to some uncertainty. Gaussian prior distributions were assigned for the oxygen feed in the five periods.

Model fitting and posterior predictive inference

The estimation of the long-term evolution of lake winter respiration and the prediction of the lake oxygen regime in future winters were used as examples of how uncertainties can be taken into account and predictions can be updated using Bayesian inference and MCMC sampling.

The benefits of Bayesian estimation were that it was possible to pool information from different sources (laboratory experiments and lake data) and to quantify the uncertainties with a full statistical approach using prior and posterior distributions. The future winters can be predicted with posterior information derived from past observations and the prior distribution. This allowed the oxygenation efficiency, for example, to be designed and controlled in order to ensure a target dissolved oxygen concentration with a given margin of safety.

The unidentifiability of the model parameters could prevent separation of their effects, but it will not hinder prediction. This is due to the Bayesian computations, which take the full multidimensional distributions of the parameters into account without resorting to linearizations or other approximations.

This simple model with a separate rate parameter k estimated for each year gave very good agreement with the winter observations (Figure 4.10) and allowed changes in respiration (Figure 4.11) and the effect of the external oxygen feed to be studied over the years.

Prior distributions for the rate parameter k, the initial O_2 concentration and the feed term can be created by pooling the posterior distributions from the past years, whereupon these prior distributions can be used to compute the predictive O_2 concentration and its prediction interval. As soon as the first observation for a winter was received, a new model with the information from the previous years as its prior

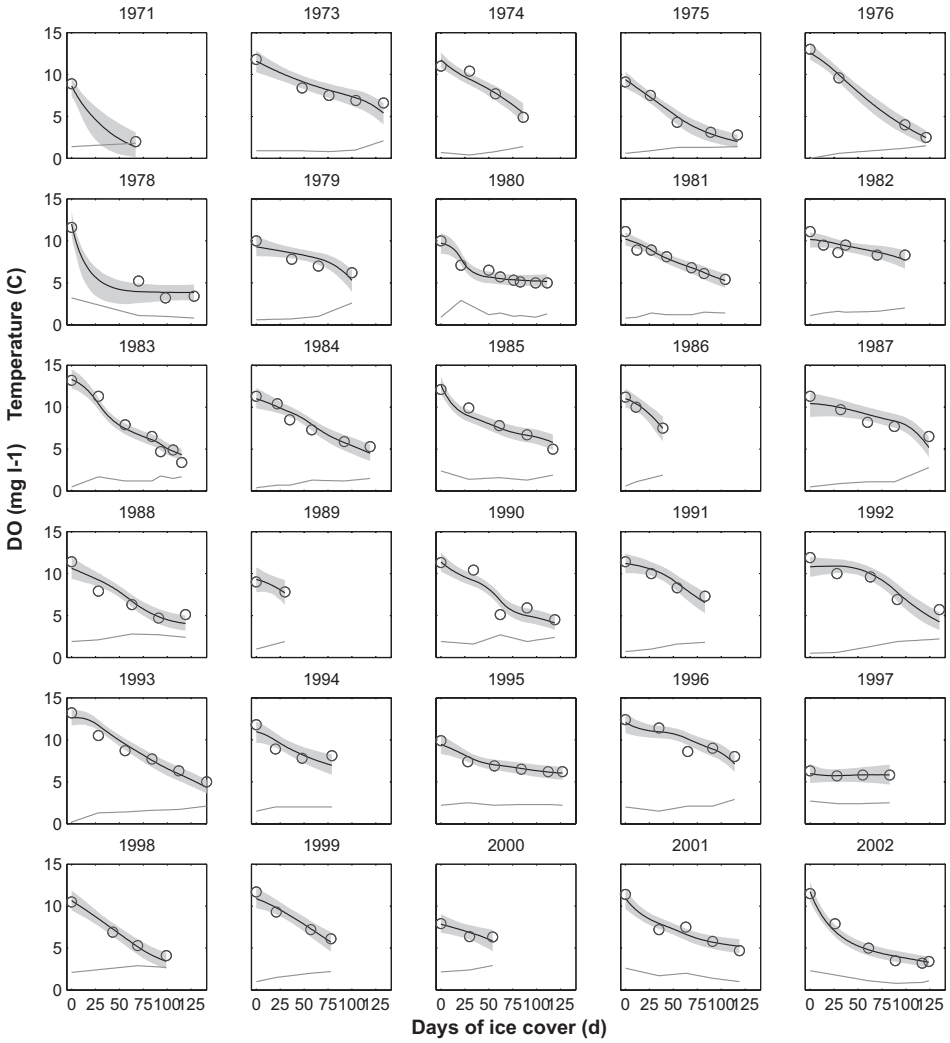

Figure 4.10: Observed oxygen concentrations (circles) $[gm^{-3}]$ and temperatures [Celsius] (lower solid line) during the ice-covered period in 1970–2000. The x-axis is time from the start of the ice-cover period. The dots represent the observed vertically averaged O_2 concentrations. The smaller dots and the dashed line show the observed temperatures [Celsius]. The solid line with a grey area around it shows the median and the 95% region of the posterior predictive distribution.

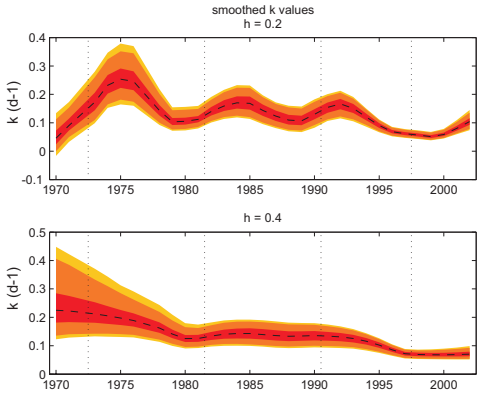

Figure 4.11: The smoothed rate constant k with two levels of smoothing. The upper plot with the lowest parameter h = 0.2 corresponds to about a 6-year trend, and the lower one with h = 0.4 to about a 12-year trend. The grey levels give 50%, 90% and 95% limits for the posterior distribution.

data was fitted and new posterior predictions were computed. The model and predictions were updated recursively with new observations (Figure 4.12).

The probability of the dissolved oxygen concentration falling below 4 mg l^{-1} was computed by predicting the concentration at the end of the ice-covered period (Figure 4.13). The empirical distribution of the length of the winter was derived from the observed lengths of the past winters.

Predictive distributions for the fresh oxygen feed needed as a function of the length of the winter (Figure 4.13) could be simulated with the Monte Carlo method. This enabled the predictions to be used for optimization and real-time process control of the aerators.

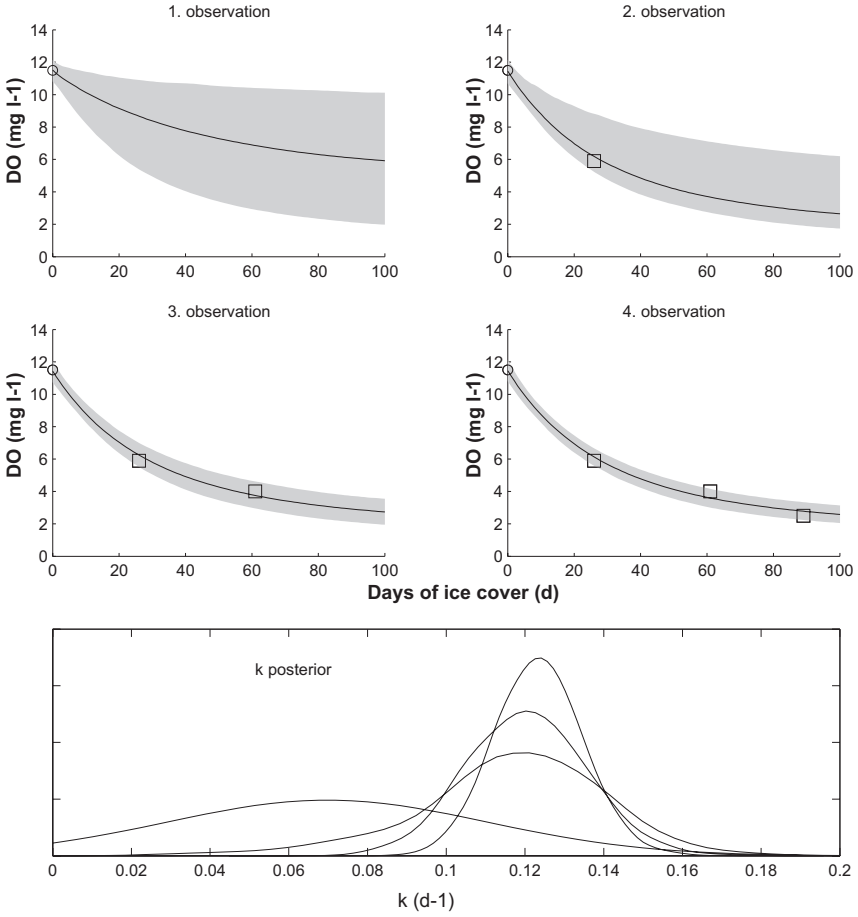

Figure 4.12: Predicting dissolved oxygen during new winter in Lake Tuusulanjärvi. The four plots in the upper part show how prediction limits for the concentration decrease as more data become available. The lower plot shows how the posterior distribution of parameter k becomes more accurate as more data become available.

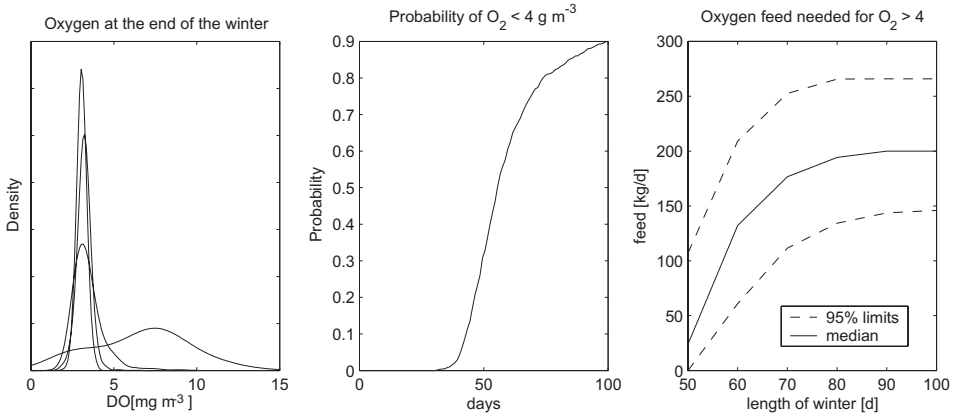

Figure 4.13: Predicting dissolved oxygen concentration in Lake Tuusulanjärvi during a new winter. The first plot on the left shows predictive posterior distributions for the amount of oxygen in the water at the end of winter. The four distributions correspond to the four observations in Fig. 4.12. The middle plot shows the probability of the concentration falling below 4 mg l^{-1} after the second concentration has been observed. The plot on the right shows how the estimated fresh oxygen feed that would be needed to keep the amount of oxygen above 4 mg l^{-1} depends on the length of the winter after the second observation.

4.5.4 Lake Pyhäjärvi in Säkylä

Prediction method

The model used for the phytoplankton dynamics in Lake Pyhäjärvi was relatively standard in specification. According to earlier trophic correlation analyses (Sarvala et al., 1998; Helminen and Sarvala, 1997), the variation in summer phytoplankton biomass in Lake Pyhäjärvi is regulated both by bottom-up (total phosphorus) and top-down (planktivorous fish and zooplankton) forces. A strong year-class of age-0+ vendace will depress the total zooplankton biomass, which in turn will reduce the grazing pressure from zooplankton, allowing an increase in phytoplankton biomass (Helminen and Sarvala, 1997). Based on these assumptions, phytoplankton was modelled with first-order reaction terms for growth, respiration, settling and death by predation (Figure 4.14). The growth rate coefficient varied in response to temperature, nutrients and light, and the non-predatory loss rate was also temperature-dependent. Temperature dependence was expressed in an exponential form, as commonly used in surface water quality modelling (Bowie et al., 1985).

The Michaelis–Menten equation was used to calculate growth limitation by total phosphorus and total nitrogen. Grazing by crustaceans was taken to be a product of the zooplankton filtration rate, crustacean zooplankton and phytoplankton biomass concentrations (Bowie et al., 1985). Temperature and half-saturation effects were omitted.

The growth and decay mechanisms were integrated into a minimal mass-balance equation for the wet weight concentration of algae A_i. Spatial variations were averaged out, and the lake was modelled as a continuously stirred tank reactor (CSTR). The use of this kind of model was supported by the earlier analyses of trophic interactions in this lake carried out by Sarvala et al. (1998). Phytoplankton was divided into three dominant groups, Diatomophyceae, Chrysophyceae and nitrogen-fixing

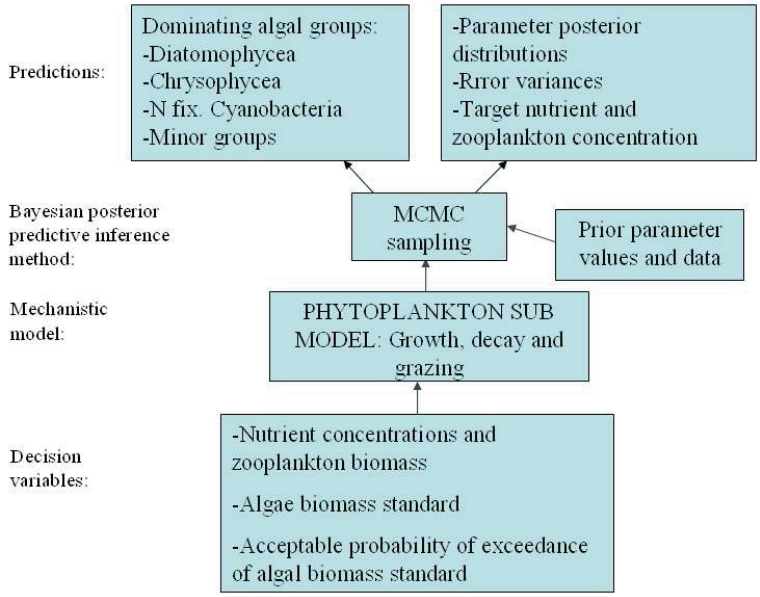

Figure 4.14: Decision variables, prediction methods and predictions for water quality management in Lake Pyhäjärvi in Säkylä.

Cyanobacteria, and an inhomogeneous group consisting of minor species.

While mechanistic water quality models tend to be overparametrized with respect to available data, the number of parameters in our water quality model was reduced. Still, there were 10 parameters to be estimated for each of the groups, in addition to which the noisy measurements of the initial spring values for each algal group in each of the eight periods were treated as unknowns. Thus, a total of 72 unknowns had to be estimated. Many of the parameters were clearly correlated, and both the control variables and the response data had high noise levels. It was obviously not possible to estimate the parameter values accurately in such a situation.

Prior distributions

Non–informative prior distributions with positivity constraints only were used for the maximum growth rates μ_i, the non-predatory loss rates σ_i and zooplankton filtration rate p_i. In addition, Gaussian prior distributions with additional positivity constraints were used for the half-saturation parameters and for the temperature coefficients θ_i based on the rather wide ranges presented in the literature (Bowie et al., 1985).

The model error ϵ_i was assumed to follow a Gaussian distribution with unknown variance, for which a standard non-informative conjugate prior distribution defined by an inverse gamma distribution was used. Separate error variances were estimated for each of the four algal groups.

Model fitting and posterior predictive inference

The parameters were estimated using eight years of water quality and hydrology observations (Figure 4.15). The parameters corresponding to Cyanobacteria (group 3) differed most clearly from the prior distributions, as these were better identified and had smaller standard deviations.

The model fits the rather noisy data relatively well, although not perfectly (Figure 4.15), and the predictive intervals for the observations cover the data reasonably well. The same set of parameters was used to model each of the eight years. The cyanobacterial blooms were predicted by the model in every year in which they were actually observed. It should be noted that the predictive intervals of the fitted model were far narrower than those of the observations.

Validation with data from five later years (Figures 4.16 and 4.17) revealed error in

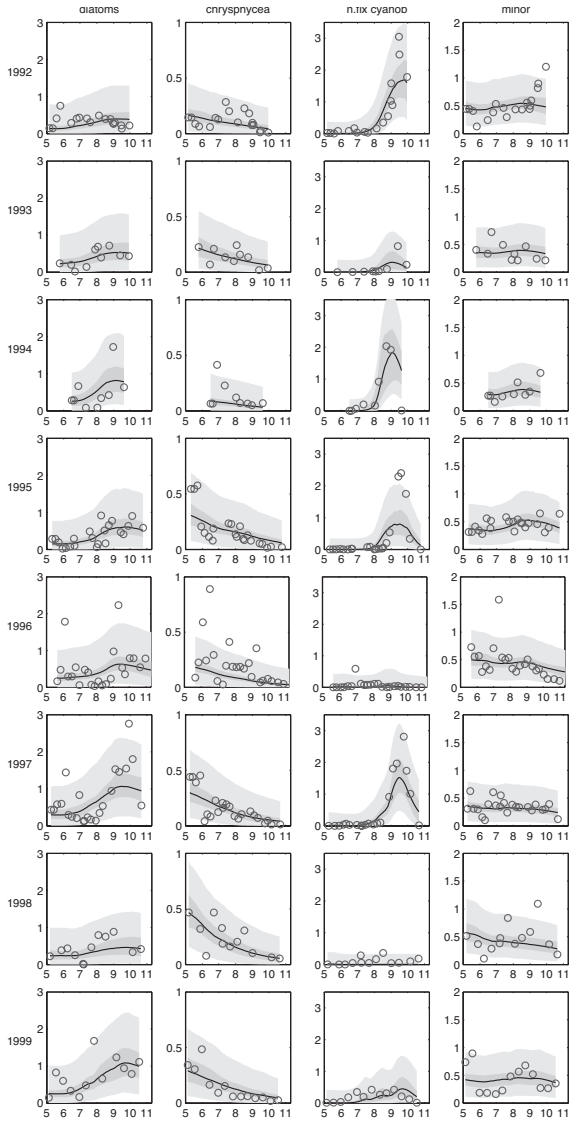

Figure 4.15: Plots of fitted models and 95 % credible intervals during the growing season. The rows represent years and the columns phytoplankton groups. Circles (o) denote observed algae wet biomass concentrations [mg l^{-1}], and solid lines show the median fits obtained by the MCMC method. The darker areas correspond to 95% posterior predictive intervals, and the lighter areas show the predictive interval for new observations. The horizontal axis shows months of the year.

the mechanistic model, since the predicted Cyanobacteria biomass in 2000 was very low compared with the observed value. Interestingly, a linear regression model for Cyanobacteria fitted to the observation for that year quite well (Figure 4.18). The data were averaged yearly and centred.

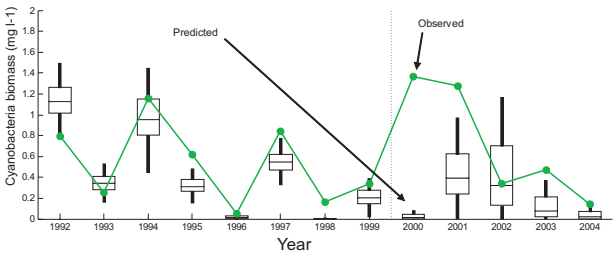

Figure 4.16: Validation of the phytoplankton model. Observed and calculated Cyanobacteria biomass in 1992–2004. Validation period 2000–2004.

The effects of zooplankton (Z), total phosphorus P_{tot} and water temperature on the mean nitrogen-fixing Cyanobacteria wet biomass concentration (A_3) during the late summer period (July 26 – September 15), were simulated using the phytoplankton model, the estimated parameters and varying control variable profiles. The simulations were performed on a grid of varying P_{tot}, Z and temp profiles and repeated with model parameters sampled from their posterior distributions and the observations sampled from their estimated distributions. The effects of biomanipulation and nutrient reduction were visualized on separate 3-dimensional probability surfaces for the different temperature profiles with averages of the P_{tot} and Z profiles on the x and y axes. The probability of exceeding the predefined water quality criteria for the mean late summer Cyanobacteria concentration (0.86 mg l^{-1}) were plotted as a response surface (Figure 4.19).

By combining the information contained in the surfaces of Figure 4.19, a more compact representation was plotted (Figure 4.20) that can be used to evaluate the limits on total phosphorus (upper limit) and zooplankton conditions (lower limit) in different mean temperatures for the attainment of the chosen water quality criteria

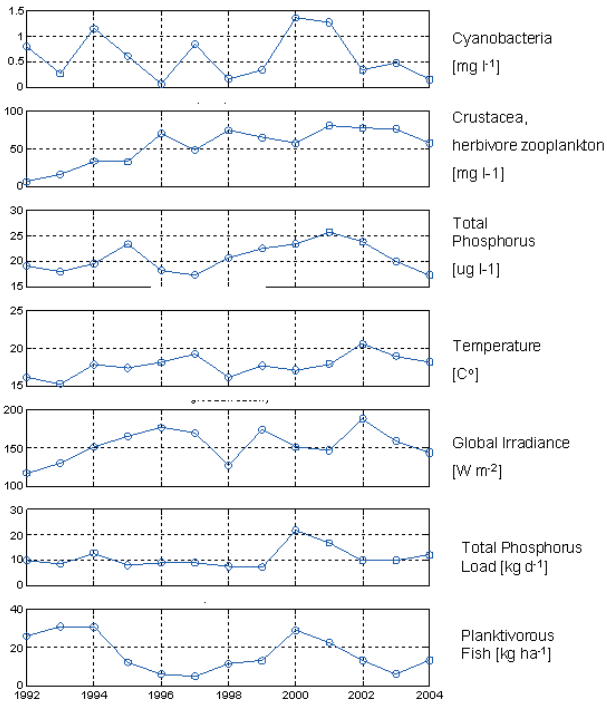

Figure 4.17: Observed control variable values in Lake Pyhäjärvi for calibration (1992-1999) and validation (2000-2004) of the phytoplankton model.

with a 95% probability. The calculated limits indicated that more zooplankton is needed to compensate for the effects of increasing temperature and total phosphorus and to fulfil the Cyanobacteria criteria laid down here. Within the observed range, total phosphorus had a marginal effect on Cyanobacteria compared with grazing by zooplankton, although the phosphorus effect increased slightly with temperature (Figure 4.20). These results agreed with the more qualitative results of Sarvala et al. (1998), where increased Z (due to the removal of planktivorous fish) was also seen to be more effective than a reduction in total phosphorus.

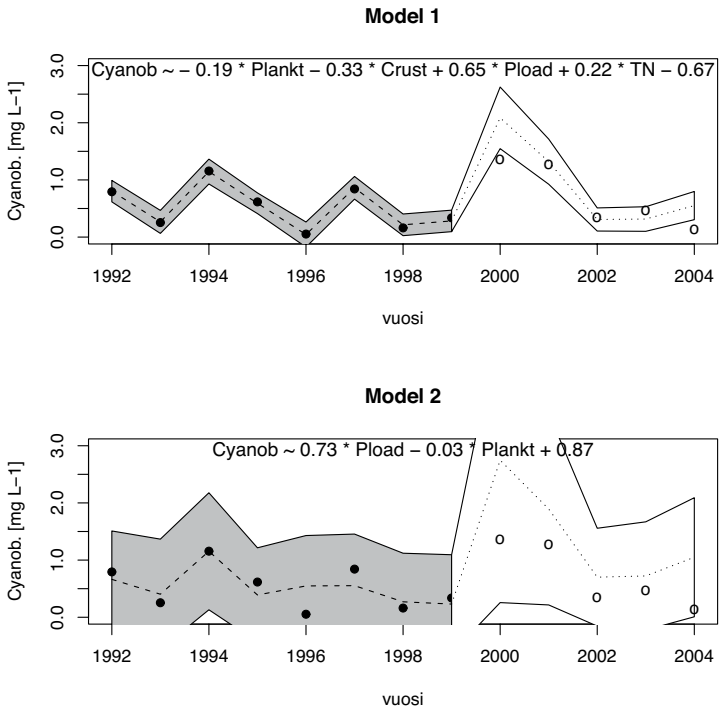

Figure 4.18: Calibration (1992-1999) and validation (2000-2004) of two optional Cyanobacteria models. Model 1 fitted best with the yearly averaged and centred data. Model 2 was designed for lake management. Variables: Cyanob - biomass of nitrogen-fixing Cyanobacteria [mg l^{-1}], Plank - planktivorous fish [$kg\ ha^{-1}$], Crust - herbivore zooplankton [$mg\ l^{-1}$], Pload - total phosphorus load [kg d^{-1}], and TN - total nitrogen concentration [μg l^{-1}].

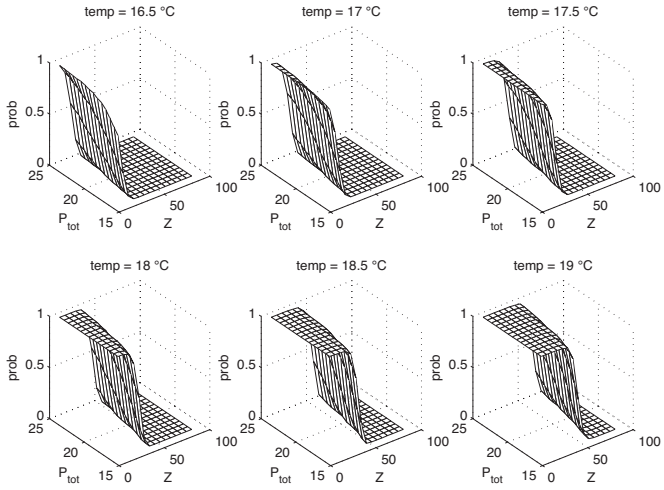

Figure 4.19: Probability of the summer mean Cyanobacteria level being greater than 0.86 mg l^{-1}. P_{tot} - total phosphorus concentration [μg l^{-1}], temp - water temperature [C^o], and Z - grazing zooplankton biomass concentration [μgC l^{-1}].

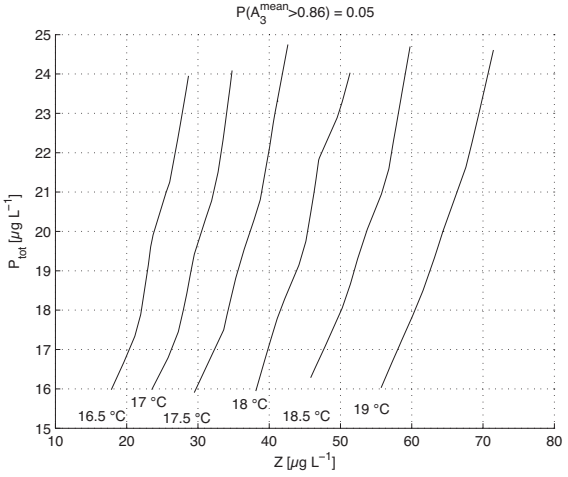

Figure 4.20: Control variable limits on exceeding a summer mean Cyanobacteria concentration of 0.86 mg l^{-1} with 0.05 probability. Each line denotes a different mean temperature profile. P_{tot} - total phosphorus concentration [μg l^{-1}] and Z - grazing zooplankton biomass concentration [μgC l^{-1}].

Integration of lake and catchment models

Later on, Bayesian inference and MCMC methods were applied to the total phosphorus and nitrogen models for Lake Pyhäjärvi, and the fitted model was combined with the phytoplankton model and a non-point load model that simulated the influences of buffer strip width, wetland percentage and forestation on total phosphorus leaching from the catchment area into the lake (Saloranta et al., 2004).

The estimated posterior parameter distributions in the nutrient models closely correlated and the credible intervals of the predictions were quite high (Figure 4.21). The phosphorus model fitted to the data better than did the nitrogen model.

Monte Carlo simulation was performed on the estimated parameter distributions and observed distributions of the control variables (wind velocity, discharge, total phosphorus and total nitrogen loading, water temperature and global irradiance) in order to estimate the impacts of nutrient loads and fisheries management on the probability of a mass occurrence of Cyanobacteria, the random variability caused by parameter uncertainty and the natural variability in the controlling variables. The resulting model was used to predict the consequences of fisheries management and a reduction in loading and to find an optimal combination of these measures with respect to the given target summer maximum Cyanobacteria biomass.

To incorporate natural variability into the predictions, samples of control variables were taken from observed 30-year time series using the bootstrap method, adding some artificial variability to the observed fluctuation in nutrient loadings and grazing zooplankton biomass in order to extrapolate their impact on the probability of a mass occurrence of Cyanobacteria. This extra variability was obtained by multiplying the loadings and zooplankton biomass by random variables sampled from the uniform distributions [0.5 1.5] and [0.1 2.0] respectively. In each simulation the model was first run to cover 20 years, in order to reach an equilibrium between

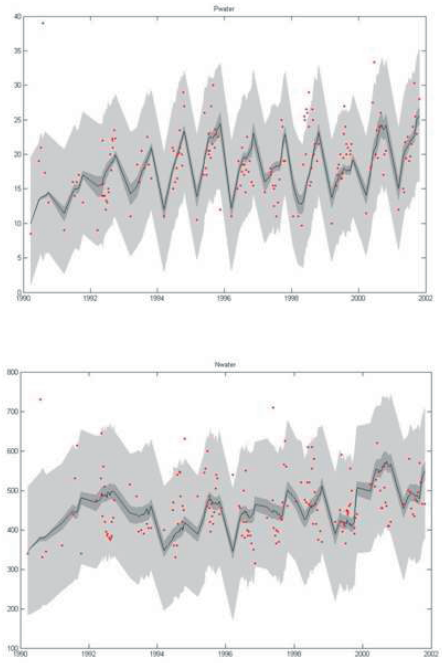

Figure 4.21: Observed and fitted nutrient concentrations [μg l^{-1}] and loads [kg d^{-1}] in Lake Pyhäjärvi in 1980-2001. Total phosphorus is in the upper plot and total nitrogen in the lower one. The nutrient models were fitted using Bayesian inference and MCMC methods. The darker grey area corresponds to the 95 % predictive limits of the fitted model, the solid line denotes the median algae concentration, and the lighter grey area gives the 95 % prediction limits for the observations.

nutrient load and lake concentrations, and was then continued for 10 more years to give a sample of predictive variables (nutrient concentrations and algal biomass).

The MC sample was used to calculate a density estimate for mean total phosphorus and maximum summer Cyanobacteria biomass conditioned on a set of total phosphorus loading and zooplankton biomass (summer maximum) ranges. The levels of external phosphorus loading and zooplankton biomass that could attain the target summer maximum Cyanobacteria biomass with the given margin of safety (90 % percentile in this example) were then estimated on the basis of these calculations.

It is also easy to calculate all the necessary percentiles for average total phosphorus concentrations and summer maximum Cyanobacteria biomasses as a function of the MC-sampled combinations of these parameters (Figure 4.22). Such results can be used to find the optimal combination of TotP load reduction and zooplankton biomass with the given range of certainty.

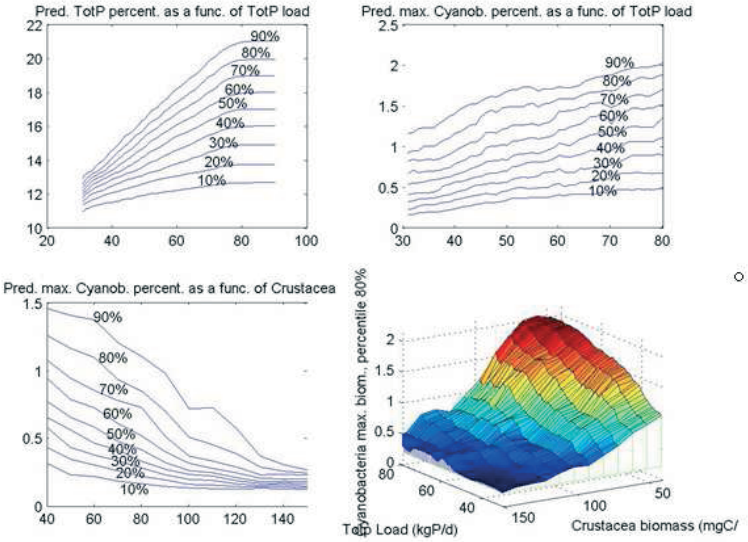

Figure 4.22: Estimated total phosphorus and summer maximum Cyanobacteria biomass percentiles (10% – 90%) as a function of total phosphorus load and summer maximum grazing zooplankton biomass. (a) mean total phosphorus percentiles as a function of total phosphorus load; (b) Max. summer Cyanobacteria biomass as a function of total phosphorus load (zooplankton biomass summer maximum fixed to a level of [30 50] mgC l^{-1}; (c) Max. summer Cyanobacteria biomass as a function of zooplankton biomass (total phosphorus load fixed to the level [30 40] kg d^{-1}); (d) Summer maximum Cyanobacteria biomass 80 % percentile as a function of total phosphorus load and summer maximum grazing zooplankton biomass. This response surface can be used to optimize nutrient load reduction and fisheries management.

In addition, Bayes network software HUGIN (www.hugin.com) was used (Saloranta et al., 2004) to learn causal relationships and conditional probability tables based on the Monte Carlo simulations of the lake model and a non-point load model (Figure 4.23) and to estimate attainment of the designated water quality criterion (Cyanobacteria summer maximum biomass < 0.86 mg l^{-1}) with a set of designed

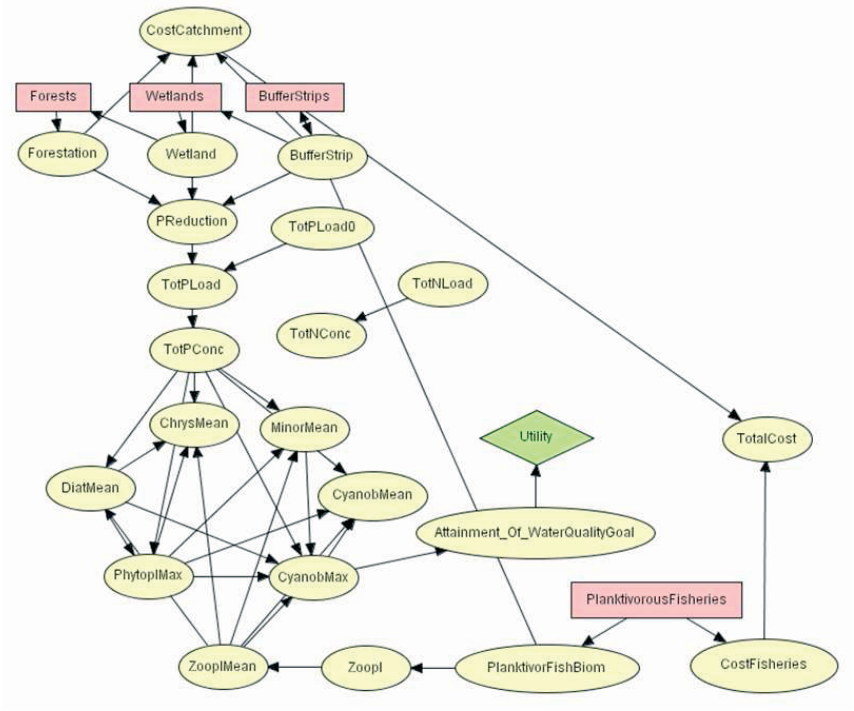

Figure 4.23: Impact diagram for management decisions in Lake Pyhäjärvi. This diagram combines the lake and catchment nutrient transport models and can be used to estimate statistical relationships with respect to the most important decision variables (rectangles) and their expected utilities (parallelogram) in terms of attainment or non-attainment of the water quality criterion (Cyanobacteria < 0.86 mg l^{-1}).

management options: buffer strip width, wetland percentage, forestation percentage and planktivorous fish management. The management options were implemented by means of decision nodes and attainment of the water quality goal with a discrete change node and a utility node that relates a certain value to each of the states of the parent nodes, in this case 1 for attainment and 0 for non-attainment of the water quality goal.

The Bayes network, decision nodes and utility nodes together formed an impact

diagram which could be used to study management decisions and their expected utilities in terms of Cyanobacteria summer maximum biomass and attainment of the water quality criterion (Cyanobacteria < 0.86 mg l^{-1}, Figure 4.23). The postulated fisheries management scenario (catch of fish 6-12 kg ha^{-1}) combined with moderate catchment measures yielded a high probability (0.779) of attaining the water quality criterion.

4.5.5 Finnish lakes

Prediction method

The predictive model for lake chlorophyll *a* (chla) concentrations was constructed on the assumption that the parameters for all lakes of the same type are likely to be similar. Therefore the estimates for these parameters can be expressed in terms of a common prior distribution. In other words, it was assumed that lake-specific model parameters are random variables representing a common distribution for the lake type. Computationally, it is natural to model the data hierarchically. That is, individual observations of chlorophyll *a* concentration are made conditional on lake-specific parameter values, which are in turn conditional on lake-type-specific parameters, which again are conditional on a parameter distribution for all lakes in Finland (Figure 4.24). Details of the Bayesian hierarchical modelling approach can be found in Gelman and Hill (2006). Qian et al. (2004) indicated that the use of a hierarchical modelling approach to pool data from different sources often results in reduced model uncertainty and improved accuracy in the parameters estimated.

The hierarchical linear model for chlorophyll *a* may be summarized as follows:

$$\begin{aligned}
\log(y_{ijk}) &\sim N(X\beta_{ij}, \tau^2) \\
X\beta_{ij} &= \beta_{0,ij} + \beta_{1,ij} \times \log(TP_{ijk}) + \beta_{2,ij} \times \log(TN_{ijk}) + \\
&\quad + \beta_{3,ij} \times \log(TP_{ijk}) \times \log(TN_{ijk}) \\
\beta_{ij} &\sim N(\beta_i, \sigma_i^2) \\
\beta_i &\sim N(\beta, \sigma^2)
\end{aligned} \tag{4.4}$$

where $\log(y_{ijk})$ is the kth observed log(Chla) value from lake j of type i, X is the matrix containing the observed total phosphorus (TP) and total nitrogen (TN)

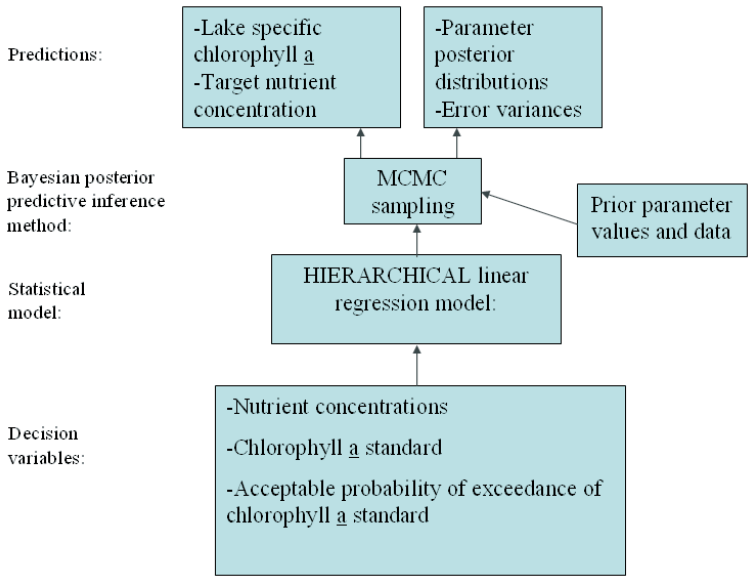

Figure 4.24: Decision variables, prediction methods and predictions for water quality management in Finnish lakes.

values from lake j of type i, $\beta_{\mathrm{ij}} = [\beta_{0,\mathrm{ij}}, \beta_{1,\mathrm{ij}}, \beta_{2,\mathrm{ij}}, \beta_{3,\mathrm{ij}}]$ is the lake-specific model parameter vector which consists of the intercept ($\beta_{0,\mathrm{ij}}$) and slopes for log(TP) ($\beta_{1,\mathrm{ij}}$), log(TN) ($\beta_{2,\mathrm{ij}}$) and for the combined effect of log(TP) and log(TN) ($\beta_{3,\mathrm{ij}}$), τ^2 is the model error variance, $\beta_{\mathrm{i}} = [\beta_{0,\mathrm{i}}, \beta_{1,\mathrm{i}}, \beta_{2,\mathrm{i}}, \beta_{3,\mathrm{i}}]$ is a vector of the model parameter means for lake type i, $\sigma^2_{\mathrm{i}} = \left[\sigma^2_{0,\mathrm{i}}, \sigma^2_{1,\mathrm{i}}, \sigma^2_{2,\mathrm{i}}, \sigma^2_{3,\mathrm{i}}\right]$ is a vector of variances in model parameters between lakes of type i, and $\beta = [\beta_0, \beta_1, \beta_2, \beta_3]$ and $\sigma^2 = [\sigma^2_0, \sigma^2_1, \sigma^2_2, \sigma^2_3]$ are the means and variance for lake types. Note that the hierarchical notation in equations 1-4 indicates conditional distributions, i.e. $\mathrm{y}_{\mathrm{ijk}}$ is normally distributed conditionally on $\mathrm{X}\beta_{\mathrm{ij}}$ and τ^2, β_{ij} is normally distributed conditionally on $\beta_{\mathrm{i}}, \sigma^2_{\mathrm{i}}$, and β_{i} is normally distributed conditionally on β, σ^2. The interaction term was added to the model to account for the non-additive effects of total phosphorus and total nitrogen.

The Markov chain Monte Carlo simulation (MCMC) method Gilks et al. (2001) was

used for estimating the distribution parameters simultaneously by sampling them from their joint posterior distribution.

Prior distributions

The non-informative prior distributions of β, $\tau, \sigma_{\mathrm{i}}$ and σ were:

$$\begin{aligned} \beta &\sim N(0, 10000) \\ \sigma_i, \sigma, \tau &\sim \mathrm{U}(0, 100) \end{aligned} \tag{4.5}$$

where $\mathrm{N}(0, 10000)$ is the normal distribution of β with mean 0 and variance 10,000 and $\mathrm{U}(0, 100)$ is the uniform distribution of $\sigma_{\mathrm{i}}, \sigma$ and τ with lower (0) and upper (100) limits. The prior distributions for σ_i, σ, τ_i and β are considered non-informative or vague. The width of the 95% credible interval for the prior distribution of β is approximately ± 200, i.e. it is practically flat in the region of interest. The standard non-informative prior distribution for a variance parameter is $\mathrm{p}(\sigma^2) \propto 1/\sigma^2$, which arises from assuming that the log of the variance parameter has a uniform distribution on $(-\infty, +\infty)$. This prior distribution is improper, which could lead to an improper posterior distribution. Instead, we used a uniform distribution for the standard deviation, as suggested by Gelman et al. (2005).

Model fitting and posterior predictive inference

The hierarchical chlorophyll a model was compared with the non-hierarchical type of specific dummy variable model and with the linear lake-specific model. Fits for four selected lakes were computed to illustrate the differences between the models

and to show the effect of the sample size on fit and on the credible interval of the prediction. The selected lakes were Lake Onkilampi - (shallow humic lake, type 8), Lake Nurmijärvi (large non-humic lake, type 1), Lake Kuhajärvi - (shallow non-humic lake, type 7) and Lake Päijänne - (large humic lake, type 2). The numbers of observations for each lake were three, seven, 22 and 265 respectively. The comparison was in general overwhelmingly in favour of the hierarchical model rather than the non-hierarchical, type-specific model. The median Chlorophyll a concentrations predicted using the hierarchical model were usually closer to the observed Chlorophyll a values than were the means predicted using the non-hierarchical dummy variable model (Figure 4.25), suggesting that the hierarchical model fits the data far better. This was also indicated by the R^2 which was greater for the hierarchical model, while the deviance and DIC of the hierarchical model were smaller than that for the non-hierarchical dummy variable model, indicating that the increased number of parameters in the former was more than compensated for by the improved fit.

When using the non hierarchical lake type–specific dummy variable model, all the lakes within one type were treated as the same and their individual observations were pooled. This model represented a weighted average with the weights proportional to the sample size for each lake, i.e. it was weighted heavily in favor of lakes with larger sample sizes. Consequently, the resulting model may be grossly biased as far as lakes with small sample sizes are concerned. This feature was clearly illustrated in the four selected lakes (Figure 4.25), where the hierarchical model treated those of the same type as exchangeable and fitted lake-specific parameters for them, but these parameters were assumed to come from the same prior distributions, thereby pooling the information from similar lakes. This pooling of information reduced the bias at the lake level and reduced the error variance as well.

The lake-specific non–hierarchical linear models were fitted using only data for a specific lake. Despite the better fit of the non-hierarchical lake-specific model relative

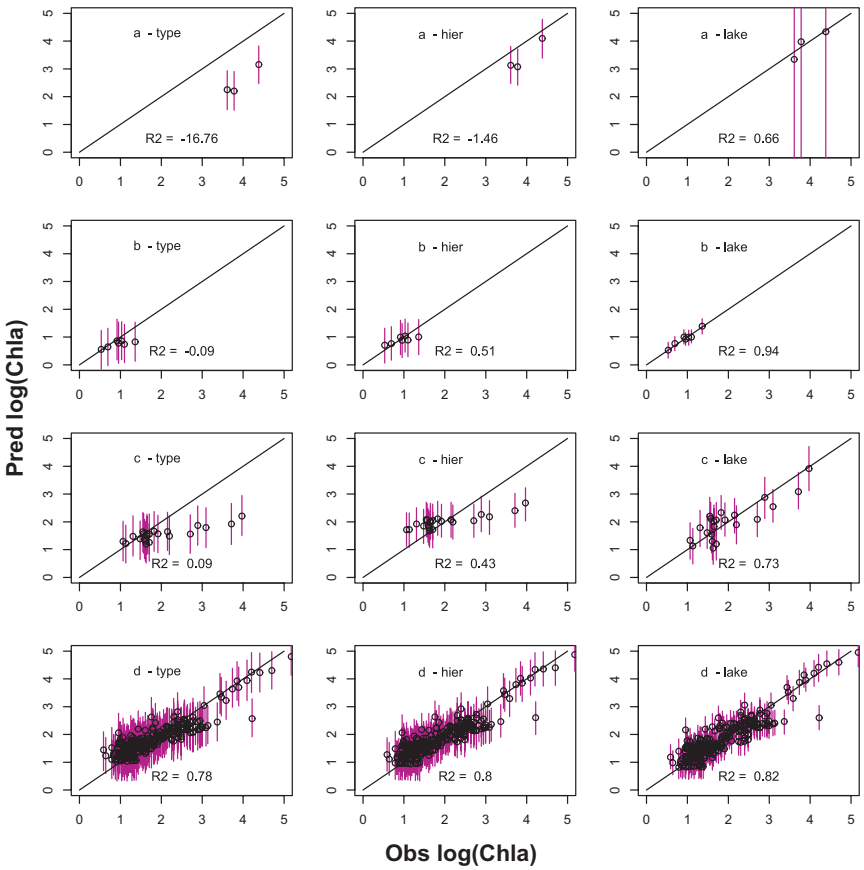

Figure 4.25: Fit plot. 10 %, 50 % (circle) and 90 % percentiles of predicted Chlorophyll a concentration [μg l^{-1}] as a function of the observed value for four selected lakes: a. Lake Onkilampi – (shallow humic lake, type 8), b. Lake Nurmijärvi (large non-humic lake, type 1), c. Lake Kuhajärvi – (shallow non-humic lake, type 7) and d. Lake Päijänne -(large humic lake, type 2). The line at a 45° angle is the 1–1 line (perfect fit). Percentiles were calculated with the lake type-specific non-hierarchical model(type), the hierarchical linear model (hier) and the lake-specific non-hierarchical model (lake). 10 % and 90 % percentiles are connected with vertical lines (linear – grey, solid line).

to its counterparts, its error variance tended to be large when the sample size was small but decreased as the sample size increased (Figure 4.25).

Lake-specific 80% percentile contour lines for Lake Päijänne (large humic lake, type 2) simulated with the hierarchical model (Figure 4.26) revealed the usefulness of posterior simulations for water quality management. The simulations were confined to the observational ranges of total phosphorus and total nitrogen in large humic lakes (type 2, TP: 2–160, TN: 31–4400), which are below the lake-specific maximum values (TP: 150, TN: 2000). The simulation in Figure 4.26 included total nitrogen values outside the lake-specific observational ranges (TP: 6–150, TN: 300–2000), but extrapolation was reasonable in this hierarchical setting due to the pooling of information within and among the lake types. This was a distinct advantage compared with the non-hierarchical lake model, which can predict only within lake-specific observational ranges. This range can be limited for lakes with only a few observations. The contour lines for Lake Päijänne were parallel to the y-axis in the observational range, showing clear total phosphorus limitation of Chlorophyll a with this range. On the other hand, total nitrogen limitation seemed to prevail near the low total nitrogen boundary and in the high total phosphorus range. A lake manager would be able to read off from figures similar to Figure 4.26 nutrient concentrations that comply with Chlorophyll a standards with a given credible interval.

The effects of total phosphorus and total nitrogen were also illustrated in the predictive plots (Figure 4.27)). The simulated Chlorophyll a increased with total phosphorus, but not very much with total nitrogen. The 10%–90% percentile predictive intervals seemed rather wide at first glance, but they were designated as credible for individual observations, since the credible interval is always wider than the commonly presented fitted confidence interval for the mean. The predictive distribution is directly related to the process of lake eutrophication assessment, while the fitted mean is not.

As the co-linearity of total phosphorus and total nitrogen makes it difficult to determine their effects on Chlorophyll a from the estimated slopes alone, posterior simulations for the Lake Päijänne (large humic lake, type 2)(Figure 4.26 & 4.27) were calculated. These showed very clear total phosphorus limitation within the observational range, indicating accurate separation of the effects despite the high correlation (0.7) between the coefficients β_1 and β_2. The co-linearity was not transferred to the predictions.

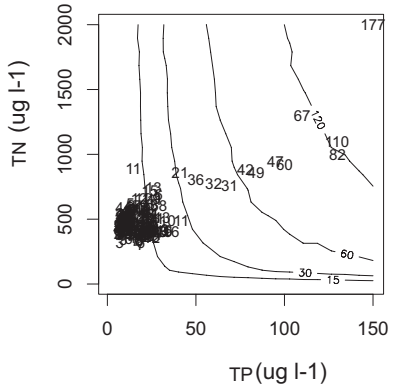

Figure 4.26: 80 % percentile contour lines for predicted Chlorophyll a concentrations in Lake Päijänne (large humic lake, type 2) at 15, 30, 60, 120 μg l^{-1} as a function of observed total phosphorus and total nitrogen concentrations [μg l^{-1}]. The predictions were simulated with the hierarchical linear model. Numbers are observed Chlorophyll a concentrations [μg l^{-1}].

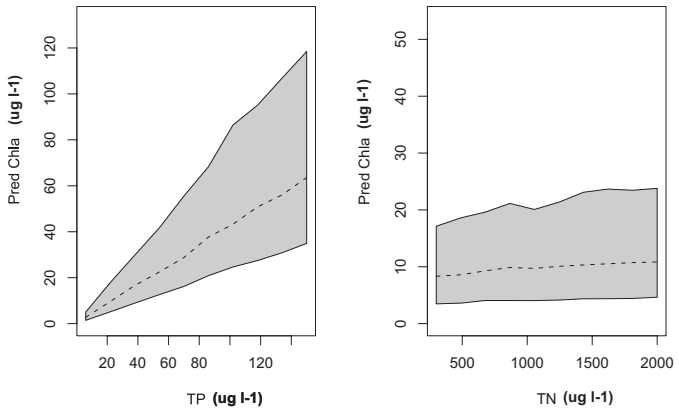

Figure 4.27: Predicted chlorophyll a concentration [μg l^{-1}] as a function of total phosphorus and total nitrogen concentration [μg l^{-1}] for Lake Päijänne (large humic lake, type 2), predicted with the hierarchical linear model. (50 % percentile - dotted line and 10 % – 90 % percentile credible interval – solid lines.) Total nitrogen is kept constant (50% percentile) while total phosphorus is varied within the observed range, and vice versa.

5 Attainment of prediction objectives

5.1 Case–specific objectives

The objectives of prediction differed greatly between the cases studied here (Table 5.1). The aim at first was to predict water quality responses to reductions in pollutant loading and to plan management actions as efficiently and realistically as possible. Later on, Bayesian inference and MCMC methods were adopted for estimating prediction errors without linearization (Figure 1.2) typical of classical least-square methods. The small size of the water quality samples in the lake monitoring data available suggested that complex mechanistic models would prove inefficient for practical river basin management purpose despite the ease of applying MCMC methods, and therefore Bayesian inference and MCMC methods were applied only to the water quality submodels at first. Later on, the nutrient model was fitted to data from Lake Pyhäjärvi by Bayesian methods, and was combined with the phytoplankton model to predict Cyanobacteria biomass as a function of nutrient load. A hierarchical chlorophyll a model for the Finnish lakes was developed in order to meet the need for a simple and efficient prediction method for use in river basin management.

5.2 Efficiency in river basin management

The applications of the prediction methods developed here will be evaluated in the following paragraphs on the basis of the case studies and the criteria for predictive scientific theories as summed up by Peters (1991). The selected criteria highlight the efficiency and predictive power of a scientific theory and reject exhaustive causal explanation of the natural processes involved as an objective for useful scientific

Table 5.1: Attainment of case-specific prediction objectives

Case	*Objective*
Lappajärvi	– Calculation of target phosphorus load given a chlorophyll a standard – Setting up a criteria for restoration dredging
Kymijoki	– Prediction of dioxin migration during and after the planned restoration dredging
Tuusulanjärvi	– Adaptive, real time control of artificial oxygenation efficiency given a dissolved oxygen standard and a acceptable probability of exceeding it – Pooling of cross-sectional information – Realistic error estimation
Pyhäjärvi	– Posterior predictive inference of target nutrient concentration and zooplankton biomass given a algae biomass standard and a acceptable probability of exceeding it – Pooling of cross-sectional information – Realistic error estimation
Finnish lakes	– Posterior predictive inference of target phosphorus loading given a chlorophyll a standard and a acceptable probability of exceeding it – Pooling of cross-sectional information – Realistic error estimation

theories. It was assumed that water quality prediction is ideally based on such theories. The criteria of Peters (1991) were:

- Relevance - focus on the management question in hand.
- Practicability - direct applicability to decision making.
- Generality - a small number of loose preconditions and applicability across a greater range of predictor variables.
- Efficiency of effort - amount of information obtained with the least effort. Effort is the cost required to perform the measurements and make and apply the predictions.
- Heuristic power - capability for inspiring debate on management options.
- Quantification - ease of deciding the accuracy and precision of the predictions.
- Accuracy - similarity between predicted and measured mean values.
- Precision - narrowness of the confidence interval (credible interval in Bayesian terms).
- Immediacy - a small number of intermediates necessary for relevant prediction.
- Simplicity - minimization of mathematical treatment and structure.

The successes and failures of the predictions in the five management cases studied here were evaluated according to the preceding criteria (Table 5.2). The majority of the predictions did indeed focus on management questions (relevance), but the chlorophyll a prediction failed in this respect because the link between nutrient concentrations and nutrient loads that would have been needed for targeting nutrient load reduction in Finnish lakes was lacking.

The direct applicability of the mechanistic prediction models for Lake Lappajärvi and the River Kymi to decision making (practicability) was limited by the lack of proper error estimates. Sensitivity analysis was used as a surrogate to rule out the risk of the migration of dioxin in the case of restoration dredging. The other predictions entailed comprehensive and realistic error estimates, but the applicability of the predictions for Finnish lakes was limited for the same reasons as their relevance.

A small number of loose preconditions and their applicability over greater ranges of the predictor variables (generality) were distinctive in the case of oxygen prediction in Lake Tuuslanjärvi and chlorophyll a prediction in the Finnish lakes. The other predictions were derived from a number of initial and boundary conditions and parameter values.

The highest amount of information for the least observational and computational cost (efficiency) was obtained using the simple prediction models for Lake Tuusulanjärvi, Lake Pyhäjärvi and the Finnish lakes, whereas the complex mechanistic models yielded information but at a substantial computational cost.

The capability for inspiring debate on management options (heuristic) was acceptable in the case of all the predictions, though the complexity of the mechanistic models for Lake Lappajärvi and the River Kymi made it hard for non-specialists to track the entire causal chain.

The accuracy (similarity between predicted and observed values) of all the predictions was reasonable, but precision (narrowness of the credible interval) was not estimated for the mechanistic models for Lake Lappajärvi and the River Kymi, so that the quantification of predictions could be said to have been insufficient. In contrast, the precision of the phytoplankton predictions for Lake Pyhäjärvi and the chlorophyll a predictions for the Finnish lakes was low, but the most important thing was that it was estimated realistically.

The criteria of immediacy (a small number of intermediates necessary for relevant prediction) and simplicity (minimization of mathematical treatment and causal deduction) were well implemented in the simple predictions for Lake Tuusulanjärvi, Lake Pyhäjärvi and the Finnish lakes, whereas the complex causal models for Lake Lappajärvi and the River Kymi included many intermediary variables and processes.

The predictions for Lake Lappajärvi and the River Kymi had the lowest sum of scores (Table 5.2), but the simulation ofthe mass and energy balances and the large amount of information included in them were of relevance for river basin management. By contrast, the simple models for Lake Tuusulanjärvi, Lake Pyhäjärvi and the Finnish lakes together with the Bayesian inference and MCMC sampling methods resulted in better scores. In the end, the criteria for predictive scientific theories proved to be a useful guide for the development of prediction methods for river basin management.

Table 5.2: General efficiency of predictions. Scores (1 = success, 0 = fail) are assigned for the selected criteria of predictive scientific theories (Peters, 1991).

Characteristic	*Value*				
	Lappajärvi	River Kymi	Tuusulanjärvi	Pyhäjärvi	Finnish lakes
Pred. variable	Chla	Dioxin	O_2	Algae	Chla
Stat. inference	-	-	MCMC	MCMC	MCMC
Number of pararam.	53	33	4/year (69)	11/species (72)	4/lake (9206)
Number of variables	11	4	1	4	1
Number of factors	8	7	2	6	2
Criterion					
Relevance	1	1	1	1	0
Practicability	0	0	1	1	0
Generality	0	0	1	0	1
Efficiency	0	0	1	1	1
Heuristic	1	1	1	1	1
Quantification	0	0	1	1	1
Accuracy	1	1	1	1	1
Precision	-	-	1	0	0
Immediacy	0	0	1	1	1
Simplicity	0	0	1	1	1
Sum	3	3	10	8	7

6 Discussion

6.1 Significance of the developed prediction methods

Implementation of the EU Water Framework Directive has initiated unparalleled administrative preparations for restoring surface waters to a good ecological status. Legislative demands for the sustainable use of surface waters have increased, river basin planning as adopted in Finland according to the EU Water Framework Directive has altered the objectives and implementation of water quality management, and new pollutant load controls that achieve the enhanced standards have had to be planned, approved, executed and updated every six years in the catchment areas of hundreds of lakes and rivers.

On the other hand, the efficiency of water quality predictions representing different levels of mechanistic and statistical sophistication has not been examined systematically before, and water quality predictions using Bayesian posterior predictive inference and MCMC methods have rarely been implemented in river basin planning or decision making (Adams, 1998). From now on, these prediction methods can be applied to river basin planning with a better knowledge of their capacity and limits. The MCMC methods that were used for the posterior simulation of predictive distributions will be particularly useful in the adaptive management suggested for the implementation of the EU Water Framework Directive (Saloranta et al., 2003), providing updated predictions that are directly applicable to the adaptation of river basin management plans and decisions.

6.2 Benefits and limitations

Large predictive errors make river basin planning and decision making difficult for without efficient prediction methods the risks remain beyond control and wrong decisions may be made (NRC, 2001). The Bayesian posterior predictive inference methods tested here enabled the prediction errors to be estimated more realistically than with classical least-square methods and first-order error analysis.

Longitudinal (lake-specific) water quality predictions and river basin management decisions are often based on either cross-sectional (observations from many lakes) or longitudinal (observations from one lake) monitoring data, with the result that they tend to be inaccurate or imprecise (wide credible intervals) (Qian et al., 2004). Bayesian posterior predictive inference and hierarchical linear regression models were used here as a remedy, to facilitate the pooling of cross-sectional information and to make the lake-specific predictions more accurate and precise.

Simple statistical prediction is often fast, easy, inexpensive and the most effective way of determining a predictive relationship (NRC, 2001; Brun et al., 2001; Reichert and Vanrolleghem, 2001). Predictions made using overparametrized mechanistic models without realistic error estimates did not score well in the present assessment of efficiency (Table 5.2), showing their inability to ensure success in management. The simple statistical predictions scored much better, indicating that complicated mechanistic prediction methods are unreasonably difficult and expensive to apply.

Model confirmation is a very complicated issue and requires a considerable number of observations, as it is believed that check runs with data not used in fitting the model will offer the best means of revealing structural errors and limitations in a mechanistic model. Besides the huge data requirements, the difficulty of coding, fitting and validation of mechanistic models reduces the efficiency of mechanistic modeling approach in a river basin management context. Moreover, measuring

campaigns need to be comprehensively and well designed in order to provide water quality predictions that are relevant in river basin management (Kettunen, 1993; Reichert and Vanrolleghem, 2001; Brun et al., 2001). Unfortunately, a comprehensive validation of mechanistic models is a luxury that is seldom achieved, due to the overparametrization of models with respect to given data and sample size (NRC, 2001; Reichert and Vanrolleghem, 2001; Brun et al., 2001). In contrast, the computational cost and data need per lake of analyzing the two thousands Finnish lakes with a hierarchical regression model was very low. Thus, simple models that are easily substantiated are preferable as demonstrated here.

The implementation of MCMC runs may be more difficult, as there is always the question of convergence of the MCMC chain to consider. This question is particularly important when dealing with a model having a large number of parameters. Parameter correlation and overparametrization increase these problems still further (Haario et al., 2001, 2004, 2003). Nevertheless, adaptive MCMC methods speeded up handling of the convergence considerably.

7 Conclusions

This study provided a new, complete statistical error analysis method for water quality prediction which facilitates realistic error estimation, the pooling of cross-sectional information for the purposes of lake or river-specific prediction and the updating of predictions. As a result, river basin planning can be based on efficient, flexible and realistic prediction methods.

7.1 Main findings

The main findings were:

- The realistic estimation of error in predictions is a prerequisite for effective river basin management.
- Realistic error estimates for mechanistic water quality predictions can be obtained using Bayesian posterior predictive inference and MCMC sampling methods.
- The accuracy and precision of water quality prediction can be improved using Bayesian inference and a hierarchical model which pools cross-sectional information for lake-specific predictions.
- Bayesian inference and MCMC methods are no more difficult to implement than classical statistical methods. Even models with large numbers of correlated parameters can be fitted using modern computational methods.
- Simple empirical models are efficient for river basin management, indicating that complex mechanistic models are unreasonably difficult and expensive to apply.

7.2 Water quality prediction, monitoring and river basin management

Guidelines were set up for water quality monitoring, prediction and river basin management in order to cope with a large number of lakes and rivers using relatively small sample sizes.

River basin monitoring should be designed statistically using the prediction error of the water quality model as an objective function. This will maximize the information value of water quality observations and minimize the prediction error. In addition, national networks for monitoring diffuse pollutant loads should be established instantly in order to meet the pressing needs of river basin management. Without determined monitoring efforts, water quality predictions will be biased and river basin management may fail to maintain the sustainable use of water resources.

Prediction is ideally implemented using Bayesian inference, MCMC methods and a simple hierarchical model. The complexity of existing mechanistic water quality models should be simplified in order to reduce their computational costs and large data requirements.

A river basin management decision should be based on a method of statistical inference that takes account of all the prediction errors realistically. This will allow progress towards the sustainable use and management of river basins to be efficiently maintained.

7.3 Continuation of research

The potential of prediction has not yet been fully realized in river basin management. For example, a prediction model can be used for the statistical design of observations in order to maximize their information value (Kettunen, 1993). Disregard of this possibility has resulted in inefficient observations and imprecise predictions. This feature will be even more important for the updating of river basin plans every six years. The continuous updating of predictions and river basin plans along with continuous monitoring constitutes an adaptive management procedure that facilitates continuous learning and correction of the courses of action adopted on the way to achieving agreed water quality goals. The statistical design of measurement protocols should be integrated into water quality prediction and management in order to galvanize the development of adaptive management strategies. The Bayesian posterior predictive inference methods introduced in this study provide new possibilities for this kind of development – not least for the statistical updating procedure, which is an intrinsic part of Bayesian inference. The use of simulated response surfaces should be developed further to allow response surface methods to be applied to river basin planning and to make good use of past and future monitoring data. The use of MCMC methods in the present instance was limited to water quality models of a single water body, but in order to enhance the utility of predictions for river basin management, their application should now be extended to cover entire river basins and a wider range of restoration techniques.

The inferential statistics developed in this study help in drawing conclusions and making predictions on the basis of limited information, but statistical decision making can go further. In addition to prediction, it can helps in revising management actions and monitoring programmes and in choosing among a number of alternative forms of river basin management. Its full potential (Raiffa and Schlaifer, 2000; Winkler, 2003) for river basin management remains to be explored.

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Glossary

Bayesian (posterior predictive) inference is a branch of statistical inference that permits the use of prior knowledge for assessing the probability of model parameters in the presence of new data. Bayesian inference has been termed 'subjective' inference, because it allows a certain subjectivity in the selection of the prior distribution and the prior distribution can greatly affect the posterior distribution (the results). Bayesian inference is also regarded as a useful tool for the exploratory analysis of data and as a way of rigorously comparing sets of assumptions. The use of prior distributions nevertheless necessarily implies a greater responsibility on the part of the researcher for ensure that no unintentional biases are introduced into the results through such prior distributions.

Burn-in is needed in Markov chain Monte Carlo sampling, where the sampled values are not independent. During a 'burn-in' period, the Monte Carlo averages converge towards the target distribution. Samples of parameters taken after the 'burn-in' period are used to estimate the posterior distribution.

Ecological status Good ecological status is defined in Annex V of the Water Framework Directive in terms of the quality of the biological community and the hydrological and chemical characteristics. As no absolute standards for biological quality can be set which apply across the Community, due to ecological variability, only a slight departure from the biological community which would be expected under conditions of minimal anthropogenic impact is allowed.

Hierarchical model linear modeling (HLM) also known as multi-level analysis, is a more advanced form of multiple linear regression. ANOVA with random effects is a simple example of hierachical linear model. Multilevel analysis allows variance in outcome variables to be analysed at multiple hier-

archical levels, whereas in multiple linear regression all effects are modelled as occurring at a single level. Thus, HLM is appropriate for use with lake water quality data which are nested within lake types or ecoregions.

MCMC sampling Markov chain Monte Carlo sampling is a stochastic algorithm for drawing samples from a posterior distribution so as to obtain an estimate of the distribution. MCMC generetes samples from an unknown probability distribution that is known up to a normalizing constant. Typical example is the posterior distributions of model parameters. As the value of the unknown constant can be given as multidimensional integral, MCMC algorithm can also be seen as a way to evaluate high dimensional integrals, a task which is computationally very demanding by any other means.

Mechanistic model is a tool for water quality prediction. Mechanistic models were first constructed in the 1970's according to a causal understanding of the phenomenon concerned and a mathematical process description. They were sometimes accompanied by least-squares parameter estimates, approximate first-order error analysis, Monte Carlo analysis or Kalman filtering. The error term attached to the model was usually neglected in prediction, and the lack of proper error estimates was compensated for by a comprehensive mathematical process description.

Model calibration or fitting includes the selection of the model (its functional form), the estimation of the model parameters as well as the errors, and their validation. It is a part of the inferential statistics used to model patterns in data, account for randomness and draw inferences regarding larger populations. In classical inferential statistics, point estimation involves the use of sample data to calculate a single value which is to serve as a best guess for an unknown population parameter. Point estimation should be contrasted with Bayesian methods of estimation, where the goal is usually to compute posterior distributions for the parameters and other quantities of interest. The contrast here is between estimating a single point (point estimation),

versus estimating a probability density function.

Posterior distribution The posterior probability distribution (or posterior probability density) is the entity for which an MCMC analysis attempts to obtain an estimate. The posterior distribution is the probability distribution over the parameter state space, given the data in the chosen model.

Posterior predictive distribution is a posterior distribution on model predictions given previous observations. It reveals all sources of uncertainty in water quality prediction and can be simulated using Monte Carlo methods and based on the MCMC chain of model parameters and on the statistical distribution of observed control variables.

Posterior simulation entails performing repeated predictions with sampled parameter values from the posterior distribution and the distributions of measured environmental conditions. Posterior simulations of the effects of various environmental conditions, i.e. the control variables of the lake model, are valuable in river basin management.

Prediction Predicting a dependent variable using other explanatory descriptors which can be manipulated experimentally, or which naturally exhibit environmental variation. A predictive model is structured according to causal relationships and process descriptions based on ecological theory and experimental or observational data. In contrast, forecasting a dependent variable using other explanatory descriptors is solely based on the extrapolation of ecological structures in space and time and does not have to be based on any law of nature and may be ecologically meaningless. Forecasting may still be useful, although prediction is ideally based on causal relationships among small number of descriptors.

Prior distribution The prior probability distribution is the probability distribution over the parameter space prior to seeing the data. This represents the prior assumptions made about the probabilities of different parameter values

before the data have been analysed. The prior distribution is combined with the likelihood to yield the posterior distribution.

River basin management A river basin is managed as a natural geographical and hydrological unit instead of according to administrative or political boundaries. Under the EU Water Framework Directive a management plan needs to be established for every river basin and updated every six years.

River basin management plan This is a detailed account of how the objectives set for a river basin (ecological status, quantitative status, chemical status and protected area objectives) are to be reached within the time scale required. The plan should include the characteristics of the river basin, a review of the impact of human activity on the status of the water in the basin, estimates of the effects of existing legislation, the remaining ”gap” to be closed in order to meet these objectives; and a set of measures designed to fill that gap. Public participation is essential, i.e. all interested parties should be fully involved in the discussion of the cost-effectiveness of the various possible measures and in the preparation of the river basin management plan as a whole.

Sampling is the main function of an MCMC run. An MCMC analysis generates a series of samples from the posterior distribution. Selection of a suitable sample for study or the act of measuring are also called sampling.

Statistical model is a parametrized set of probability distributions which can be used for statistical inference in river basin management.

Target pollutant load is the flux of a polluting substance into a lake or a river that has a given probability of protecting a selected water quality standard. It should ideally be estimated using statistically designed observational data, a water quality model and inferential statistics.

Validation Runs with data that located outside the range of variation of the calibration data are used to confirm a model and to reveal structural errors

and limitations in it. In Bayesian analysis, the prior distribution is combined with data to calculate the posterior distribution, from which inferences about the parameters are made. The postulated probability model is never expected to be entirely true but is chosen in the light of the available knowledge and constructed with the simplest possible structure. It must therefore be tested at each step in the investigation. Residual quantities are calculated and sensitivity to prior distributions is tested in order to evaluate the probability model critically and to suggest modifications.

Water frame work directive "Directive 2000/60/EC of the European Parliament and of the Council establishing a framework for Community action in the field of water policy" or in short, the EU Water Framework Directive (WFD) was adopted on 23 October 2000, with the following key aims:

- to expand the scope of water protection to all waters, surface waters and groundwater
- to achieve "a good status" for all waters by a set deadline
- to implement water management based on river basins
- to introduce a "combined approach" laying down emission limit values and quality standards
- to involve citizens more closely
- to streamline the legislation
- to implement river basin management with reasonable costs.

Water quality criteria can be used to define a water quality standard, e.g. for protection against pollutants with potential ecological effects. Biological criteria, for example, describe the desired aquatic community for a water body based on the numbers and kinds of organisms expected to be present. Nutrient criteria are used to protect against nutrient over-enrichment and cultural eutrophication. Sediment criteria describe the conditions necessary in order to avoid the adverse effects of contaminated sediments.

Water quality standard form the foundation of water quality-based pollution control. They define the goals for a water body by designating its uses, setting criteria for protecting those uses and establishing provisions for protecting it from pollutants.

Summary

River basin plans in the member states of the European Union are to be updated every six years. To complete this enormous task efficiently, accurate and precise water quality predictions and realistic error estimates have to be employed. These will provide a better insight into the fate and influence of the pollutants for the designing, operation and optimization of river basin management.

Water quality prediction has traditionally been based either on mechanistic or statistical prediction models. Mechanistic models stand in for hydraulics, while statistics are mainly used for biological and chemical processes. The statistical error analysis applied to the mechanistic models using least-square parameter estimation and first-order error analysis was only approximative, however, and unrealistic. This meant that reconciliation of the methodologies was inefficient.

This thesis attempts to estimate the error in water quality predictions realistically and to unify the mechanistic and statistical prediction methods using Bayesian posterior predictive inference and MCMC sampling methods. By the same token, it alters the paradigm of prediction and decision making from deterministic to statistical. These methods proved to be useful in the real time control of artificial oxygenation devices and thus anticipated the efficiency of such an approach for the adaptation of river basin plans every six years.

Water quality predictions are usually based either on a longitudinal lake-specific sample or a cross-sectional sample from many lakes. Existing Finnish lake monitoring data are a mixture of longitudinal and cross-sectional data. Lake-specific predictions based on such data tend to be imprecise or inaccurate. This deficiency was compensated for by using Bayesian inference methods and hierarchical models, which enabled cross-sectional water quality data to be pooled efficiently in order to

ensure more accurate and precise lake-specific chlorophyll a prediction.

The evaluation of mechanistic, statistical and Bayesian prediction methods was based on extensive data from 5 water quality management cases. First, the chemical and biological responses to pollutant loads and hydrological conditions were modelled and predicted with a mechanistic lake and river model. Second, predictive uncertainties in lake respiration and phytoplankton submodels were estimated using Bayesian inference and MCMC sampling methods. This enabled deterministic water quality predictions to be transformed into predictive distributions, which were more useful for statistical decision making in the context of river basin management. Third, targets were set for pollutant load reductions for the lakes studied here and a criterion for the restoration dredging of contaminated river sediments based on the predictions.

The main findings were:

- Realistic error estimation is a prerequisite for realistic decision making and effective river basin management.
- Realistic estimates of the error entailed in mechanistic water quality predictions can be obtained using Bayesian posterior predictive inference and MCMC sampling methods.
- The accuracy and precision of lake-specific chlorophyll a predictions based on data from the Finnish lake monitoring network can be improved using a hierarchical model structure.
- Bayesian inference and MCMC methods are no more difficult to implement than classical statistical methods. Even models with a large number of correlated parameters can be fitted using modern computational methods.
- Simple empirical models are efficient for river basin management, indicating

that complex mechanistic models are unreasonably difficult and expensive to apply.

Guidelines for water quality monitoring, prediction and river basin management were set up to cope with a large number of lakes and rivers using relatively small sample sizes. River basin monitoring should be designed statistically using the prediction error of the water quality model as an objective function. This will maximize the information value of water quality observations and minimize the prediction error. In addition, national networks for monitoring diffuse pollutant loads should be established instantly in order to meet the pressing needs of river basin management. Without determined monitoring efforts, water quality predictions will be biased and river basin management may fail to maintain the sustainable use of water resources. Prediction should ideally be implemented using Bayesian inference, MCMC methods and a simple hierarchical model. The complexity of existing mechanistic water quality models should be simplified to reduce their computational costs and large data requirements. River basin management decisions should be based on a method of statistical inference that takes account of all the prediction errors. This will enable the progress being made towards the sustainable use of water resources to be efficiently maintained.

Yhteenveto

Huonokuntoisten vesistöalueiden hoitosuunnitelmat tullaan Euroopan unionin jäsenvaltioissa tarkistamaan kuuden vuoden välein. Tähän niitä velvoittaa vesipuitedirektiivi, joka hyväksyttiin europarlamentissa 22. joulukuuta vuonna 2000. Sen seurauksena Suomessakin vahvistettiin vuonna 2004 laki vesistöalueiden hoidon organisoimisesta. Hoidettavia, huonokuntoisia vesistökohteita on satoja, ja niiden hoitosuunnitelmat pitää olla valmiina vuonna 2009. Hyvä vedenlaatu näissä kohteissa saavutetaan nopeimmin ja pienimmin kustannuksin, jos suunnittelussa käytetään vedenlaadun ennusteita, joidenka ennustevirheet on arviointu realistisesti.

Perinteisesti vedenlaatuennusteet ovat perustuneet joko mekanistiseen tai tilastolliseen mallintamiseen. Laskentaintensiivisiä mekanistisia malleja on käytetty pääasiassa vesistöjen virtaus- ja kulkeutmisongelmien ratkaisemiseen, kun tilastollisia menetelmien käyttö on painottunut kemiallisten ja biologisten ilmiöiden analysoimiseen. Mekanistisen ja tilastollisten menetelmien yhdistäminen on ennusteiden realistisen virhearvioinnin ja vesistöjen hoidon tehokkuuden kannalta ensiarvoisen tärkeää.

Tässä työssä mekanistinen ja tilastollinen lähestymistapa yhdistettiin käyttäen Bayeslaista posterior päättelyä ja MCMC menetelmiä. Saman aikaisesti ennustamisen ja vesistöjen hoitoon liittyvän päätöksenteon periaateet muuttuivat deterministisestä tilastolliseksi.

Vedenlaatuennusteet perustuvat yleensä joko pitkittäiseen tai poikittaiseen havaintootokseen ts. havaintoihin yhdestä tai monesta vesistöstä. Sen sijaan järvien seurantaaineistolle on tyypillistä pieni järvikohtainen havaintomäärä suuresta joukosta järviä. Tällöin järvikohtaiset ennusteet ovat epätarkoja tai virheellisiä. Ennusteiden laatua saatiin parannettua hierarkisen mallirakenteen ja Bayeslaisin päättelymenetelmien avulla.

Kehitetyt mekanistiset, tilastolliset ja Bayeslaiset vedenlaadun ennustemenetelmät testattiin aineistolla viidestä vedenlaadun hoitotapauksesta. Ensiksi mekanistisilla järvi- ja jokimalleilla ennustettiin ravinnekuormitusten, kunnostusruoppauksen ja hydrologisten osoluhteiden vaikutus vedenlaatuun. Seuraavassa vaiheessa järven happi- ja kasviplankton mallien ennustevirheet estimoitiin Bayes-päättelyn ja MCMC-menetelmän avulla. Näin mekanististen mallien pistemäiset ennusteet muutettiin tilastollisiksi jakaumiksi, jotka ovat hyödyllisiä vesistönhoidon tilastollisessa päätöksenteossa. Lopuksi ennusteiden perusteella laskettiin kuormitusten ja pitoisuuksien vähennystavoitteita ja asetettiin rajoitus kunnostusruoppauksen yhteydessä liikkelle lähtevän ja dioksiinin likaaman sedimentin määrälle.

Tärkeimmät löydöt olivat:

- Vedenlaatuennuste realistinen virhe-estimaatti on tehokkaan vesistönhoidon edellytys.
- Mekanistisen mallin realistinen virhe-estimaatti voidaan laskea Bayes-päättelyn ja MCMC-menetelmän avulla.
- Suomalaiseen järviseuranta aineistoon perustuvan järvikohtaisen klorofylli a ennusteen virhettä ja epätarkkuutta voidaan edelleen pienentää hierarkisen mallirakenteen avulla.
- Bayes-päättelyn ja MCMC-menetelmän laskennallinen toteuttaminen ei ollut vaikeampaa kuin klassisten tilastomatemaattisten menetelmien toteuttaminen. Jopa suuren määrän korreloituneita parametrejä sisältävä vedenlaatumalli saatiin sovitettua havaintoaineistoon.
- Yksinkertaisen empiirisen mallin tehokkuus vedenlaadun ennustamisessa ja vesistönhoidon suunnittelussa osoittaa, että monimutkaiset mekanistiset mallit voivat joskus olla kalliimpia ja työläämpi kuin tarpeellista.

Työssä annettiin yleisluonteisia, vedenlaadun seurantaa ja ennustamista sekä vesistöalueiden hoitoa koskevia ohjeita, joissa kiinnitetään erityistä huomiota suurten vesistöalueiden hoidon suunnitteluun suhteellisen pienten havaintoaineistojen ja tässä työssä kehitettyjen menetelmien perusteella. Lisäksi ehdotetaan hajakuormituksen kansallisen havaintoverkoston perustamista ja liittämistä toiminnallisesti yhteen em. kokonaisuuden kanssa havaintoaineistojen riittävän informaatiosisällön varmistamiseksi vesistöjen hoitotoimien suunnittelun ja päätöksenteon kannalta.

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