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344

**Niina Kotamäki**

# Statistical Methods for Adaptive River Basin Management and Monitoring

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## ABSTRACT

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Decision-making at different phases of adaptive river basin management planning rely largely on the information that is gained through environmental monitoring. The aim of this thesis was to develop and test statistical assessment tools presumed to be particularly useful for evaluating existing monitoring designs, converting monitoring data into management information and quantifying uncertainties. River basin scale monitoring was performed using a wireless sensor network and a data quality control system and maintenance effort was assessed. National-scale, traditional monitoring data and linear mixed effect modelling were used to estimate the uncertainty in two status class metrics (total phosphorus, and chlorophyll-a) by quantifying temporal and spatial variance components. The relative sizes of the variance components were then used to determine how to efficiently allocate the monitoring resources. Nutrient and chlorophyll-a statuses were linked to external loading utilizing a large amount of monitoring data and a hierarchical Bayesian approach. This linkage was the basis for developing a practical assessment tool for lake management. To evaluate the network of relationships affecting phytoplankton development between water quality variables, structural equation modelling was used. Model residual and parameter uncertainty, and thus uncertainty in the assessment result, were estimated using probabilistic Bayesian modelling. In general, the results of this study suggest that the used statistical methods appear to be particularly useful for decision-making under an adaptive management framework, as they enabled predictions to be made based on existing monitoring data and have measures of uncertainty associated with the outcomes. The results suggest that the uncertainties often stem from the lack of input data or insufficiently allocated monitoring. Therefore, it should be ensured that information gaps in the nutrient loading values, as well as in other, especially biological variables, are sufficiently covered.

Keywords: Adaptive management; Bayesian inference; eutrophication; monitoring; statistical methods; uncertainty; Water Framework Directive.

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# CONTENTS

## LIST OF ORIGINAL PUBLICATIONS

This thesis is based on the following original papers, which will be referred to in the text by their Roman numerals I–V.

I was the corresponding author in I, and responsible for the automatic quality control system, data warnings and data compilation for evaluating the network and maintenance performance. Sirpa Thessler wrote the first version of I. I had the main responsibility in planning II and III. I was also responsible for the first drafts and carried out the statistical analyses and modelling. In IV and V my main role was on statistical and methodological aspects, and co-author contribution to the text and improving it. Papers III-V have been included in the PhD thesis by Anita Pätynen (Pätynen 2014). Her emphasis was on ecological aspects, and she performed the literature search and review in V and wrote the first versions of IV and V.

I Kotamäki N., Thessler S., Koskiaho J., Hannukkala A.O., Huitu H., Huttula T., Havento J. & Järvenpää M. 2009. Wireless in-situ sensor network for agriculture and water monitoring on a river basin scale in Southern Finland: evaluation from a data user's perspective. *Sensors* 9(4): 2862–2883.

II Kotamäki, N., Järvinen, M., Kauppila, P., Korpinen, S., Lensu, A., Malve, O., Mitikka, S. and Kettunen, J. A practical approach to improve statistical performance of WFD monitoring networks. Manuscript.

III Kotamäki N., Pätynen A., Taskinen A., Huttula T. & Malve O. 2015. Statistical dimensioning of nutrient loading reduction - LLR assessment tool for lake managers. *Environmental Management* 56: 480–491.

IV Pätynen A., Kotamäki N., Arvola L., Tulonen T. & Malve O. 2015. Causal analysis of phytoplankton development in a small humic lake using structural equation modelling. *Inland Waters* 5: 231–239.

V Pätynen A., Kotamäki N. & Malve O. 2013. Alternative approaches to modelling lake ecosystems. *Freshwater Reviews* 6: 63–74.

# 1 INTRODUCTION

## 1.1 Background and problem setting

Aquatic ecosystems are an important natural resource and ecosystem service. They provide both provisional use of the waters, and recreational and cultural benefits. The concern about the condition of aquatic ecosystems has become more prominent over the past decades. Changing climate, anthropogenic pressures and new emerging pollutants have led to the deterioration of the status of the surface waters (Hering *et al.* 2015). To ensure sustainable use of water resources and the ecosystem services they provide requires protecting, enhancing and conserving the condition of the watercourses (Hallett *et al.* 2016). Concrete water management policies, processes and guidelines are set by legislation. There are several examples of legislative drivers at the national level: the US Clean Water Act (CWA), the South African National Water Act (NWA) and the Australian and New Zealand National Water Quality Management Strategy (NWQMS); binational: Great Lakes Water Quality Agreement (GLWQA) and on a multinational level: the European Water Framework Directive (WFD) and the Marine Strategy Framework Directive (MSFD). There are clear similarities between the US CWA approach and the European water management as both are based on the idea of aiming at the attainment of predetermined water quality standards (Hallett *et al.* 2016). The quality standards are based on several indicators and dependent on the characteristics of the watercourse.

Environmental monitoring produces information to answer designated assessment and management questions (Loucks and van Beek 2005). Efficient use of the monitoring data provides a scientific background for decision making when assessing the condition, pressures, changes and causal relationships in aquatic ecosystems. For supporting water management many monitoring methods, such as traditional water sampling, remote sensing, biomonitoring, continuous water quality sensors and large-scale wireless sensor networks, produce data that have different spatial and temporal resolutions. Despite the method of data collection, it is important to evaluate the quality of the data and ensure that they provide representative information about the water quality. This way it becomes possible to control the pressures through suitable management actions. Continuous, on-line water quality measurements have been seen as a promising way to gain more accurate nutrient loading estimates (Horsburg *et al.* 2010, Tattari *et al.* 2017). In addition, to gain more precise information, variability over time and space is necessary to quantify when planning efficient monitoring designs (Loucks and van Beek 2005) or evaluating existing programmes (Levine *et al.* 2014). This is because the required sampling frequency in time and the number of monitoring sites depend on the ecosystem variability.

Changing environmental stress, societal demands and policy needs require constant adaptation of management and monitoring to answer the right questions and to meet current complex challenges (Lindenmayer and Likens 2009, Lindenmayer *et al.* 2012). In addition, aquatic ecosystems are generally very dynamic, and their variability and responses are hard to predict (Williams 2011). This introduces uncertainty which makes it difficult to estimate the effects of alternative scenarios and select the best management actions (Pahl-Wolst 2007). Uncertainties can be estimated, e.g., by using the Bayesian modelling approach. The general philosophy behind the Bayesian approach is that the model parameters themselves follow some statistical (probability) distribution (Gelman *et al.* 2002). This feature means that the uncertainties related to model parameters can be explicitly defined. Bayesian models are also adaptive in the sense that their parameters, error variance, and thus their predictions can be updated when new information is gained. This is because the Bayesian approach facilitates the use of other information than just the current data. This information is known as prior information and it reflects the previous knowledge about the model parameters obtained, e.g., from previous studies or data. The prior information, expressed as a prior distribution is combined with the data which results in a posterior distribution. As estimating the posterior distribution is often complex and its exact form is unknown, the use of Markov Chain Monte Carlo (MCMC) or similar simulation tools are often used to solve this problem (e.g., Gilks *et al.* 2001).

Mathematical models are necessary to support, supplement and integrate water management (Rekolainen *et al.* 2003, Loucks and van Beek 2005). Different modeling strategies, such as deterministic process-based models and statistical data-driven methods are complementary, and they are suitable for different scales and situations. Statistical methods are especially needed to plan data sampling, convert the data to information and to quantify uncertainty (Anon. 2001). There is a particular need for assessment methods that i) account for the uncertainty in the results, ii) are applicable on different scales, and iii) use monitoring data efficiently (see, e.g., Hering *et al.* 2010).

## 1.2 River basin management planning (II, III, IV)

In 2000, the EU Water Framework Directive (WFD) (2000/60/EC) was implemented aiming at achieving good ecological and chemical status in all EU waterbodies. The WFD's management approach is not based on national boundaries but on river basins, which are natural geographical and hydrological formations. Implementing the WFD is an iterative process where the member states have to deliver river basin management plans (RBMP) every six years to set out how to improve their water resources to achieve a good status. The first RBMPs were adopted in 2009 covering the implementation plans for 2009−2015 and the second in 2015 covering the years 2016−2021. The third management cycle ends in 2027 and at present it defines the final deadline for meeting the WFD objectives towards the good status of the waters. For the management plans, rivers, lakes and coastal waters have to be assessed, their pressures identified, programmes of measures (PoMs) set, and the impacts of the PoMs need to be evaluated.

The status assessment is the base for defining and targeting the management measures. The WFD ecological status assessment is strongly based on a range of biological quality elements (phytoplankton, macrophytes, phytobenthos, benthic macroinvertebrates, and fish) that are especially sensitive to key environmental pressures, such as eutrophication or changes in physical habitats (hydromorphological alteration). The waterbodies are assessed and classified into one of the five ecological status classes (high, good, moderate, poor or bad), and these classes are defined as the amount of deviation from the undisturbed (reference) conditions. The reference conditions and thus the quality standards (i.e. class boundaries) vary depending on the type of the waterbody, and for this, the waterbodies are divided into different types according to their physical and morphological attributes (Anon. 2003a). The waterbody status class of a single indicator (metric) of the biological quality element (BQE) is often estimated as an average value (mean or median) of the metric over the 6-year assessment period. The status class estimates are inevitably associated with uncertainty that should be dealt with in a systematic way (Birk *et al.* 2012, and Reyjol *et al.* 2014). Calculating the uncertainty for a status class metric can be done using statistical models and information from different sources of variability (Clarke 2013, Carstensen and Lindegarth 2016). Further, the status class uncertainty should be given as probabilities, however, these have only been taken into account in fairly few assessment systems (Hering *et al.* 2010).

In addition to the status assessment it is crucial to define the pressures that may cause the deterioration of the status. The decision whether to start PoMs is the class limit between 'Good' and 'Moderate' The predominant anthropogenic pressure in lakes and coastal areas in Europe is eutrophication which is largely caused by excessive nutrient loading from agriculture (Anon. 2012, Hering *et al.* 2015). Assessment tools for modelling loading responses and calculating the amount of nutrient loading reductions are an integral part of the RBMP (Anon. 2001). Traditionally, empirical eutrophication models (e.g., Vollenweider 1968) have been used to link the incoming nutrient loading with the in-lake nutrient concentration. These models have been considered useful predictive tools for lake management (Brett and Benjamin 2008, Shimoda and Arhoditsis 2015). A widely used indicator of eutrophication is chlorophyll-*a* (chl-*a*) concentration to measure phytoplankton biomass (Carvalho *et al.* 2008). Chl-*a* has well-documented relationships with the nutrient concentration, especially phosphorus (Lyche-Solheim *et al.* 2013). Chl-*a* reacts quickly to increased nutrient loadings thus being among the most sensitive and informative indicators for estimating the efficiency of eutrophication related management actions

## 1.3 Monitoring for RBMP (I, II, V)

Monitoring is an essential part of the management framework for gaining information to assist in decision making. The underlying questions behind any effective monitoring programme are what, where, when, and how often to measure (Gitzen *et al*. 2012). For RBMP it is important to collect enough representative data to assess the waterbody's ecological status, to characterize human impacts, and to evaluate the responses to management actions (Hirst 2008, Hallett *et al.* 2016). However, there are several stumbling blocks which undermine the reliability of the data produced by the ongoing long-term monitoring programmes. The objectives, the monitoring design and the extent of monitoring are often insufficiently considered (this is expressed in more detail in Lindenmayer and Likens 2009). Monitoring programmes have sometimes been criticized for being inefficient and lacking in focus (Lovett *et al.* 2007). It seems that all too often that time and money are invested to obtain data before sufficient consideration has been given to how the data will or could be used and what is the value of the data compared to the costs (Loucks and van Beek 2005). Furthermore, without scientific knowledge for better justification, the development of monitoring programmes is often driven by the constant pressure to reduce monitoring costs.

Currently, policy instruments, such as WFD, MSDF and the Nitrates Directive, largely steer the monitoring in Europe. For surface waters, WFD has proposed monitoring requirements for the biological, hydro-morphological and associated physico-chemical elements, especially for status assessment, identifying management needs, and targeting PoMs (Anon. 2003b). The requirements of the WFD have led to challenges for many member states to shift their monitoring programmes towards a more biologically-based and comprehensive approach (Martins *et al.* 2009, Collins *et al.* 2012). Especially in Finland and other Nordic countries, due to the high abundance of lakes, rivers, and the length of coastal waters coupled with limited resources for environmental administration, not all waterbodies can be monitored with the intensity and frequency requested by the WFD (Andersen *et al.* 2016). Therefore, there is a need to evaluate the ongoing monitoring designs and to allocate the sampling efforts optimally to produce reliable information for status classification. Allocating the monitoring resources so that the uncertainty which is caused by spatial and temporal variation is minimized will, in turn, maximize the confidence of status classification (Carstensen 2007).

The increased importance of the water management and the need for more spatially and temporally accurate data has speeded up the development and testing of new monitoring techniques. These techniques include, e.g., wireless sensor networks for monitoring water quality and weather parameters at the catchment level (Porter *et al.* 2005, Ojha *et al.* 2015). Such sensor networks produce spatially and temporally accurate data from several sites and for multiple parameters. The data can be used for many purposes and to answer multiple research questions related to water quality and quantity (see e.g. Seders *et al.* 2007 and Kido *et al.* 2008). Especially for water management issues, water quality sensors together with continuous water level information at the river mouths produce reliable nutrient loading estimates (Jones *et al.* 2012). More accurate loading estimates are important in areas where nutrient-enrichment is particularly a problem. However, even though sensor networks produce useful information, they also pose challenges for data quality control and network maintenance (Porter *et al.* 2005).

## 1.4 Adaptive monitoring and management

The constant changes in environmental stress, social demands and thus also the management objectives urge a more adaptive approach for the management of waterbodies. The concept of adaptive management (Fig. 1), which is a broad 'learning from experience' type of framework, is well described in the scientific literature (see e.g. Holling 1978, Pahl-Wostl 2007, Williams 2011). As an iterative learning process, adaptive management offers a framework for integrating management objectives and options, modelling, monitoring, stakeholder participation and decision making (Anon. 2004). The basic idea of adaptive management stems from the fact that the natural ecosystems are complex and unpredictable and their responses to management actions are largely uncertain (Anon. 2011). Because of this uncertainty, there is a need to gain more knowledge about the relationships, and cause-effects, and to iteratively manage the system based on the new information.

The management actions should improve over time based on the information the monitoring programmes produce. Monitoring is a fundamental part of the adaptive management concept for gaining the information that is needed (Gitzen *et al*. 2012, Lindenmeyer and Likens 2009). Additionally, the monitoring should adapt changing objectives, evolving knowledge and new techniques (Fölster *et al.* 2014). However, there should also be a balance between the adaptation and securing the integrity of the long-term time-series

(Lindenmeyer and Likens 2009, Fölster *et al.* 2014). The reasons for collecting data and the accuracy of the variables of interest have to be addressed when monitoring under the adaptive management framework (Loucks and van Beek 2005).

Although adaptive management suits local scale problems well, it is usually associated with large-scale and complex applications (Williams 2011). An example of small-scale adaptive monitoring would be using adaptation in a high-frequency monitoring scheme (adaptive sampling frequency) to improve and enhance the system's capacity. Large-scale adaptive management has been adopted, e.g., in the US to estimate the total maximum daily loads of water bodies (TMDL; Reckhow 2005). The implementation of WFD sits well under a large-scale adaptive management framework as it is fundamentally an iterative learning process (Hering *et al.* 2010). The WFD requirement of maintaining and pursuing the good ecological status of European waters has shifted water management towards a more holistic and integrated approach (Kaika 2003). Statistical models have proved (Anon. 2011) particularly useful for decision making under an adaptive management framework as they enable to make predictions from the data and they have measures of uncertainty associated with the outcomes (Fig. 1).

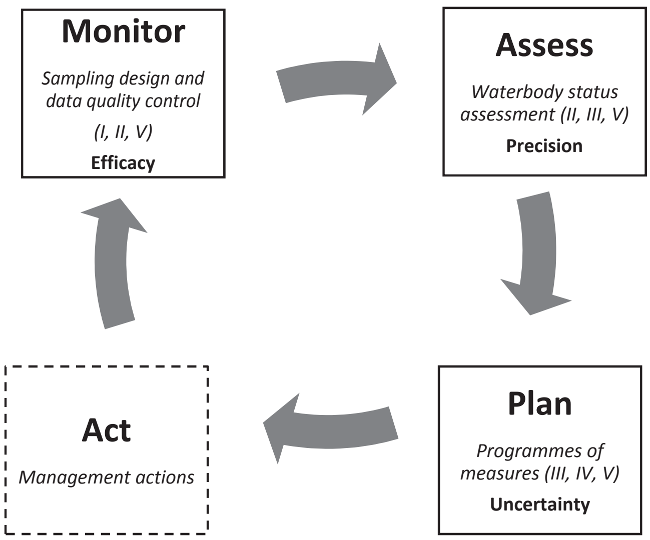


FIGURE 1 Conceptual graph of an adaptive monitoring and management cycle. Monitoring produces information for status assessment, which in turn is a base for the planning process. The plans for programmes of measures are implemented as management measures. The success of the management actions is again evaluated via monitoring and this produces the new status assessment (Modified from Stankey *et al.* 2005). The steps which are addressed in this thesis are highlighted as boxes with solid lines and the aims of this study (in bold text) are to evaluate the efficacy of the monitoring (I, II, V), the precision of status assessment (II, III, V) and the uncertainty in the loading responses (III, IV, V).

# 2 OBJECTIVES

The main objective of this study is to develop and test statistical assessment tools which would help more adaptive river basin management planning. The specific interest was to determine if these methods could support status assessment and determination of loading reductions under uncertainty at different phases of the decision-making process related to the monitoring. The more specific aims were

i) To evaluate how much maintenance and data quality control effort is needed when operating a large-scale wireless sensor network (I).
ii) To study how the sampling design affects the ecological status class probabilities and whether it is possible to better allocate the monitoring resources (II).
iii) To develop and test an assessment tool for calculating required nutrient loading reductions in lakes affected by eutrophication (III).
iv) To test and evaluate if the causal relationships in the water-related questions could be addressed with a structural equation modelling statistical method (IV, V).
v) To evaluate the uncertainties related to different assessment methods (II, III, IV)
vi) To increase the awareness of different statistical methods suitable for RBMP (V).

The wireless sensor network performance was evaluated based on the data from maintenance information and an automatic warning system (I). Due to the sparse and heterogenic nature of the long-term monitoring data and varying scales of management planning, hierarchical (II, III) and causal modelling frameworks (IV) were used for analysing the data. The applicability and usage of these methods were reviewed (V). Uncertainties in the model structures and assessment results were estimated using a Bayesian modelling framework (III, IV).

# 3 MATERIALS AND METHODS

## 3.1 Study sites and data

### 3.1.1 General description

The statistical analyses in this thesis were based on data with different spatial and temporal scales, ranging from the waterbody level to river basin and national scales (Fig. 2). The data analysed in II, III and IV are from national Finnish monitoring programmes whose data are stored in the open source database of the Finnish Environment institute (SYKE 2017). The data in II address lakes, rivers and coastal waterbodies, and in III and IV only lakes. The river basin scale data was collected during the wireless sensor network project in the Karjaanjoki river basin (I).

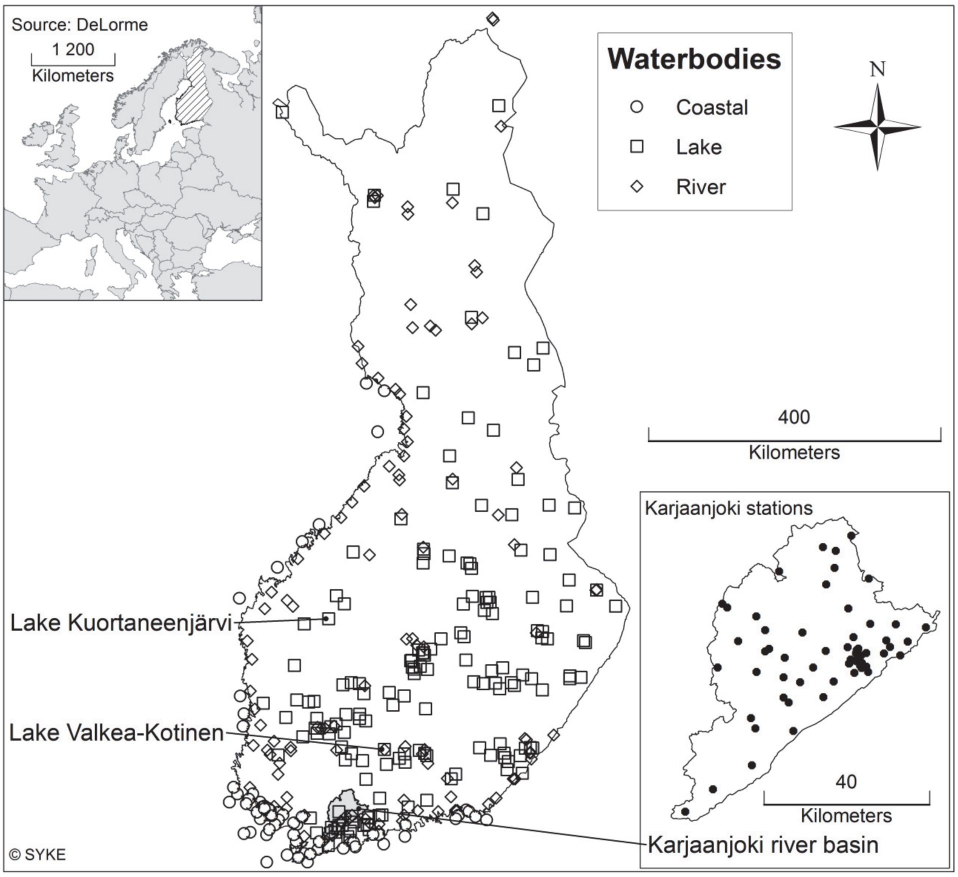


FIGURE 2 Geographical coverage of the study sites. Intensively measured coastal, lake and river waterbodies (II), Karjaanjoki sensor network (I), Lake Kuortaneenjärvi (III) and Lake Valkea-Kotinen (IV).

### 3.1.2 National scale (II, III)

The national scale studies include analyses of two (different) data sets. First, for analysing the uncertainty in the status assessment and evaluating the optimal sampling design the data from the most intensively monitored Finnish surface waterbodies were analysed (II). These data (2006−2012) include rivers ($n$ = 74), lakes ($n$ = 165) and coastal waters ($n$ = 39) that represent broadly different water body types (see Appendix in II). The chl-*a* observations from the lakes ($n$ = 6,742) are from June to September and for coastal waterbodies from July to the 1st week of September ($n$ = 1,448). For rivers, the TP concentration represents the whole year ($n$ = 10,406). The coastal data include 11 inner coastal waterbodies (connected to land), 10 open coastal waterbodies and 2 waterbodies from the middle archipelago.

TABLE 1 Status class metrics, time spans, number of waterbodies, sampling sites and observations in different water categories (II).

| | Lakes | Rivers | Coastal |
|---|---|---|---|
| Metric | chl-*a* (µg $l^{-1}$) | TP (µg $l^{-1}$) | chl-*a* (µg $l^{-1}$) |
| Sampling depth | 0–2 m | mainly 1 m or less | 0–5 m |
| Period | 2006−2012 | 2006−2012 | 2006−2012 |
| Months | Jun−Sep | Jan−Dec | Jul − 1st week of Sep |
| Waterbodies (n) | 165 | 74 | 39 |
| Sampling sites | 257 | 115 | 67 |
| Samples | 6,742 | 10,406 | 1,448 |

The other national-scale monitoring data set was formed to examine the variation in chl-*a*-to-nutrient responses between different lake types. The data included July–August 1990–2007 chl-*a*, TP and TN concentrations from 2,246 Finnish lake waterbodies with a total of 36,942 observations. The data structure was (naturally) hierarchical, as the individual observations belong to a sampling site, which in turn belongs to a water body, which are grouped to national lake types (see Aroviita *et al*. 2012).

### 3.1.3 Regional scale (I)

The aim of establishing a large-scale wireless sensor network in 2007-2008 was to establish multipurpose and multi-functional monitoring to study weather related environmental phenomena. The network was located in the Karjaanjoki river basin in south west Finland (Fig. 3). About 63 % of the 2,000 $km^2$ catchment is covered by forests and 18 % are agricultural areas. The main lakes in the area are Lake Hiidenvesi (area 29 $km^2$, mean depth 6.7 m) and Lake Lohjanjärvi (area 92 $km^2$, mean depth 12.7 m). Rivers Vanjoki and Vihtijoki transport waters to Lake Hiidenvesi from which the waters run into the Lake Lohjanjärvi along the River Väänteenjoki. Finally, the waters flow into the Gulf of Finland in the Baltic Sea via River Mustionjoki.

When operating at its full capacity, the Karjaanjoki river basin sensor network hosted 77 sensor nodes. Of these, 55 were weather stations, 11 were water turbidity stations and 4 were nutrient measurement stations (measuring nitrate concentration, turbidity, water level and water temperature). In addition, there were 30 soil moisture sensors and 7 turbidity sensors connected to the weather stations. The sensor nodes were from several sensor manufacturers and the server services were provided by two different companies (for more details see Huitu 2009). Water related parameters were measured with spectrometers or optical backscatter sensors and soil moisture was measured using capacitance or reflectometry sensors. The frequency of the measurements varied from one measurement every 15 min. to one every hour.

The sensor network provided over 30,000 measurements per day and 20 million measurements during the 1.5 year evaluation period.

The sensor instrumentation covered the entire Karjaanjoki river basin and three intensive measurement areas. Management practices were tested in the Hovi farm area and the effectiveness of a constructed wetland was evaluated. The Vihtijoki sub-catchment was intensively instrumented to gain validation data for sub-catchment level hydrological modelling. Thirdly, the nutrient balance of Lake Hiidenvesi was measured with water quality monitoring sensors at the inflow and outflow of the lake. In this thesis the focus is on the data quality and maintenance evaluation. The results of the applications of paper I are not presented here.

### 3.1.4 Local scale (III, IV)

For demonstrating the use of a loading modelling assessment tool in lake management planning, the eutrophic Lake Kuortaneenjärvi (area 15 $km^2$, mean depth 3.3 m) was studied. The highly-humic lake is an important recreational lake in the Ostrobothnia region of Finland (Rautio and Aaltonen 2006). Its relatively large catchment area (1,266 $km^2$) consists mostly of peatland and forests. The lake is exposed to heavy diffuse loading especially from agriculture but also from forestry, peat production and waste waters from scattered settlements. Lake Kuortaneenjärvi is regulated and the lake acts as a natural sedimentation pond for the lower parts of the catchment. This has led to strong release of phosphorus from bottom sediments (internal loading). As a consequence of the excessive external and internal nutrient loadings the lake has become hypereutrophic resulting in cyanobacterial blooms and occasional oxygen depletion in the deepest areas. The water quality has improved, as indicated by the slightly reduced nutrient and chl-*a* levels, in the past 10 years due to long-term and active management measures. Fish removals especially have directly affected the internal loading and improved the water quality (Sivil 2006). Based on all quality elements the ecological status of Lake Kuortaneenjärvi is still moderate and an important measure to improve the (eutrophication related) status is to reduce the external loading on the lake (Westberg 2016). In this study the target nutrient loading for Lake Kuortaneenjärvi was estimated using measured TN and TP concentrations (annual averages 1991−2013). External nutrient loadings and water outflow estimates were taken from the national-level nutrient loading estimation tool Vemala (Huttunen et al. 2016). The limits and thus the targets for a good ecological status class for highly humic lake types are 20 $\mu g\ l^{-1}$ for chl-*a* , 45 $\mu g\ l^{-1}$ for TP and 750 $\mu g\ l^{-1}$ for TN (see Table 1 in III).

For studying the causal effects of phytoplankton development, Lake Valkea-Kotinen, a boreal lake with long monitoring data and active phytoplankton research was chosen. Lake Valkea-Kotinen is a small, pristine headwater lake in Southern Finland. The lake’s sheltered catchment area is dominated by forests and the lake is highly-humic and brown-coloured which also explains strong summer temperature stratification. The long-term integrated monitoring (1990−) and lack of anthropogenic pressures has made Lake Valkea-Kotinen an important reference site, especially for climate change, and brownification studies (Vuorenmaa *et al.* 2011, Lehtovaara *et al.* 2014). The dataset for analysing the relationships affecting phytoplankton development was based on weekly sampling during 1990−1995 from the central part of the lake. Due to the strong stratification and seasonality, only the summer (Jun−Aug), epilimnetic samples of chl-*a,* nutrient fractions (TP, TN, PO2, NO3 and NH4), water colour and temperature were chosen. Zooplankton counts from pooled sampling were strongly skewed and were thus transformed with natural logarithm prior to the analysis to ensure the multivariate normal assumption of the estimation methods.

## 3.2 Methodology

### 3.2.1 Sensor network maintenance and data quality control (I)

The quality of the data of the sensor network is dependent on many aspects starting from the proper deployment of the sensors and stations. Additionally, maintenance, cleaning, calibration and automatic data quality control procedures are important steps when aiming to obtain reliable and useful data. For the River Karjaanjoki sensor network, extra emphasis was placed on evaluating the maintenance effort and developing automatic quality control algorithms, especially to provide alarms for maintenance needs.

Several quality control tests were implemented to automatically detect possible errors in the sensor data (I). These tests were developed to replace earlier manual quality controls. The data quality problems that were regularly encountered included suspiciously high or low measurement values, missing data and observing the same value repeatedly. For missing data, two different tests were developed: 1) for checking long periods of missing data (over 24 hours) and 2) for occasional missing values. The third test calculates the variance of the previous values and checks that there has been variation in the measurements for the last 24 hours. These tests were carried out sequentially and the fourth test was for inspecting whether the measured value is within the predetermined range. Compared to crude range tests that the sensor manufacturers offer, this algorithm accounts for site and sensor-specific variation. For weather sensors, the Finnish Meteorological Institute provided the range limits which were based on the monthly climate extremes of the hemiboreal climatic zone. The limit values for water related parameters and soil humidity were defined based on long site-specific data records. Based on the range test every measurement was given an information label (flag) indicating whether the measurement was correct, questionable or wrong.

The tests were automatically run on a daily basis. The quality control system collected the possible warning messages on the quality checks and an e-mail notification was sent to the data quality controller who made a decision whether to inform the maintenance team or not. The maintenance effort was evaluated based on the log file where the maintenance and cleaning activities were stored. For evaluating the maintenance effort, records from a 4-month period were collected.

### 3.2.2 Variance component estimation (II)

The sampling uncertainty in the status classification is determined as the precision of the estimated metric mean and the confidence to which a water body can be assigned a status class. For assessing the mean and variance of the chl-*a* and TP status class in the intensive monitored waterbodies (Chapter 3.1.1) we used a statistical, mixed effects model. In the model the indicator is expressed as a linear sum of fixed and random variables (Pinheiro and Bates 2000, Zuur *et al.* 2009).

For the status classification of a particular assessment period, a single observation (*l*) from a year (*i*) and month (*j*) and a sampling station (*k*), can be expressed as a sum of the (fixed) overall mean ($\mu$) and the components of random variation between years ($year_i$), months ($month_j$), sampling sites ($site_k$) and unexplained residual variation ($\varepsilon_{ijkl}$) (Eq. 1). For simplicity, it was assumed that all variability is random.

$$\log(y_{ijkl}) = \mu + year_i + month_j + site_k + \varepsilon_{ijkl} \quad (1)$$

We assumed that the natural log-transformed chl-*a* and TP measurements, $\log(y_{ijkl})$, in the observed data follow a normal distribution with a mean $\mu$ and variance $\sigma^2$, denoted as $log(y_{ijkl}) \sim \mathcal{N}(\mu,\sigma^2)$. The variance components are assumed to be independent and normally distributed as follows: $year_i \sim \mathcal{N}(0,\sigma^2_{year})$, $month_j \sim \mathcal{N}(0,\sigma^2_{month})$, $site_k \sim \mathcal{N}(0,\sigma^2_{site})$ and $\varepsilon_{ijkl} \sim \mathcal{N}(0,\sigma^2_{\varepsilon})$. Because the chl-*a* and TP data were right-skewed they were log-transformed. Based on histograms the lognormality assumption was sufficiently valid. As the mean and the variance components are unknown they are estimated from the data with statistical modelling. The relative size of the estimated variance components reflects the uncertainty that stems from different sources. For comparing uncertainties between metrics, waterbodies or waterbody types, the metric precision, given as a relative standard error of the mean (RSE) is calculated from the estimated standard error divided by the estimated mean:

$$\mathrm{RSE} = \frac{\sqrt{\hat{\sigma}}}{\hat{\mu}} \cdot 100\ \% \quad (2)$$

The estimated variance components can now be used for finding an optimal sampling design in relation to the frequency and the size of temporal and spatial variation (based on Cochran 1977 and applied e.g. in Clarke 2013, Carvalho *et al.* 2013, Carstensen and Lindegarth 2016). The uncertainty of the waterbody metric mean (i.e. the total sampling variance, $\sigma^2$) can be calculated as follows:

$$\sigma^2 = \frac{\sigma_{year}^2(1-\frac{nr_{year}}{max(nr_{year})})}{nr_{year}} + \frac{\sigma_{month}^2(1-\frac{nr_{month}}{max(nr_{month})})}{nr_{month}} + \frac{\sigma_{site}^2}{nr_{site}} + \frac{\sigma_e^2}{nr_{year}nr_{month}nr_{site}n} \quad (3)$$

In our case the maximum number of years (max($nr_{year}$)) is 7 (2006-2012), maximum number of months ($max(nr_{month})$) for lake chl-$a$ is 4 (Jun–Sep), for coastal chl-$a$ 3 (Jul – 1st week of Sep) and for river TP 12 (Jan-Dec). It is possible to choose the number of years ($nr_{year}$), months ($nr_{month}$), sites ($nr_{site}$) or samples ($n$) so that the overall variance is as small as possible. For example, if the variation between sampling sites is large the overall uncertainty can be reduced by increasing the number of sites that are monitored.

The status class confidence is calculated using a normal probability distribution with the estimated metric mean and the overall uncertainty (Kelly et al. 2009, Lindegarth and Carstensen 2013). The probability of a class ($p_{class}$) depends on the status class limits for each waterbody type (see Appendix in II). Thus, the confidence of class 'High' is $100(1-p_{High})$, confidence of class 'Good' is $100(p_{Good}-p_{Moderate})$, confidence of class 'Moderate' $100(p_{Moderate}-p_{Poor})$, confidence of class 'Poor' is $100(p_{Poor}-p_{Bad})$, and confidence of class 'Bad' is $100(p_{Bad})$. These probabilities sum up to 100%.

The results of the uncertainty analysis were used for statistical rules that the decision makers can utilize in practice when reallocating the sampling resources (Fig. 3.) The overall uncertainty (RSE), confidence of the status class and the variance sources were calculated for all 272 intensively monitored waterbodies, and the statistical rules could be applied to their monitoring schemes. When the status class confidence was high (over 80 %) and the overall error low (under 20 % or 10 % depending on the status class) the sampling could be reduced according to the smallest variance component. On the other hand, based on the decision rules, the waterbodies with the most uncertain status classification need more monitoring effort.

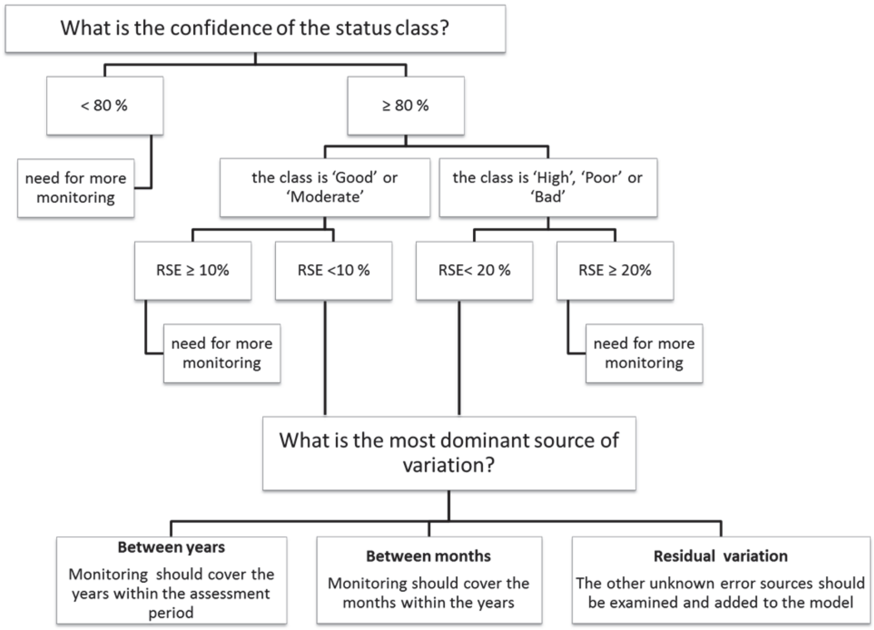


FIGURE 3 Statistical rules for aiding how to allocate the waterbody level monitoring effort in temporally optimal way.

### 3.2.3 LLR model tool for lake managers (III)

We have developed an assessment tool, called Lake Load Response (LLR), for estimating the lake-specific TP and TN loading reductions and the confidence of the status class with the given loadings. The chl-*a* concentration, a surrogate for algal biomass, is used as a biological metric. In-lake concentrations are estimated as a function of nutrient loading, outflow, sedimentation rate and the lake area following the parametrization of the well-known TP and TN mass-balance models (Vollenweider 1968, Chapra 1975, also recently reviewed in Brett and Benjamin 2008). The in-lake TP ($C_{TP}$, mg m$^{-3}$) or TN ($C_{TN}$, mg m$^{-3}$) concentration can be expressed with the TP loading ($L_{TP}$, mg d$^{-1}$) or TN loading ($L_{TN}$ mg d$^{-1}$), settling velocity ($v_s$, m d$^{-1}$) and the surface area of the lake (A, m$^2$) as follows (Eq. 4):

$$C_{TP/TN} = \frac{L_{TP/TN}}{Q_{out} + v_s A} \tag{4}$$

The external loading, concentration and outflow are from lake-specific data. The settling velocity, which is the only unknown parameter, is assumed to vary randomly according to a normal distribution with a mean $\mu_s$ and a variance $\sigma_s^2$. This is a fair assumption as the settling velocity is usually poorly defined and the input data are noisy. The model can now be formulated as follows: $C_{TP/TN} \sim \mathcal{N}(f(\mathrm{v_s}, x), \tau^2)$ and $v_s \sim \mathcal{N}(\mu_{\boldsymbol{s}}, \sigma_s^2)$. The nutrient concentrations ($C_{TP/TN}$)

follow a normal distribution ($\mathcal{N}$) with a mean $f(v_s, x)$ and variance $\tau^2$. The mean value is derived from the Vollenweider nutrient retention model (*f*) (Vollenweider 1968) with the observed lake-specific input data in vector **x**.

The estimated concentrations (and thus the link from the loadings) are associated with the lake biology (chl-*a*) through a hierarchical linear regression model fitted to large amounts of data from Finnish lakes. The model was originally developed by Malve and Qian (2006). Here we fitted the chl-*a*-nutrient response model to more recent data and used the updated lake types. The hierarchical chl-*a* model includes the overall mean for chl-*a* and the main effects of TP and TN concentrations, and their interaction and the random variability between lakes and lake types. The hierarchical chl-*a* model can be expressed as follows (Eq. 5-8):

$$\log(chla_{ijk}) \sim \mathcal{N}\left(\mathrm{X}\beta_{ij}, \tau^2\right) \tag{5}$$

$$X\beta_{ij} = \beta_{0,ij} + \beta_{1,ij}\log\left(TP_{ijk}\right) + \beta_{2,ij}\log\left(TN_{ijk}\right) + \beta_{3,ij}\log\left(TP_{ijk}\right)\log\left(TN_{ijk}\right) \tag{6}$$

$$\beta_{ij} \sim \mathcal{N}(\beta_i, \sigma_i^2) \tag{7}$$

$$\beta_i \sim \mathcal{N}(\beta, \sigma^2) \tag{8}$$

Here $chla_{ijk}$ is chl-*a* concentration of sample *k* from lake *j* of lake type *i* and matrix X contains the observed TN and TP values from the lake. Parameter vector $\beta_{ij}$ consists of the lake-specific intercept ($\beta_{0,ij}$), log(TN) and log(TP) slopes ($\beta_{1,ij}$, $\beta_{2,ij}$) and their interaction ($\beta_{3,ij}$). Lake type specific parameters are analogously expressed as vector $\beta_{ij}$ and the global scale parameters as vector $\beta$. The beta parameters can be seen as fixed effects (see Chapter 3.2.3), contributing to the mean chl-*a*, and the $\tau^2$ and $\sigma^2$ contribute to the variation. See also the notifications in Malve and Qian (2006) (and II).

The applicability of the LLR tool to a single lake was demonstrated for Lake Kuortaneenjärvi (Chapter 3.1.4). The effect of external nutrient loading and associated uncertainties were estimated.

### 3.2.4 Structural equation modelling (IV, V)

To evaluate a network of relationships affecting phytoplankton development between water quality variables in Lake Valkea-Kotinen structural equation modelling (SEM) was used. SEM, also known as causal modelling and analysis of covariance structures, is a highly flexible and broad methodological framework (Kline 1998). SEM has been rarely used for aquatic ecosystems even though it provides a promising tool for complex water management issues, where the effects between physical, chemical and biological variables can be indirect and causal, these variables are often correlated and error-contaminated, and the assumptions of traditional methods are not met (Arhonditsis 2006). SEM explicitly incorporates measurement errors (uncertainty) in all variables and allows the use of so called latent variables that are not directly measured, but they constitute of multiple indicator variables that conceptualize a theory of interests (e.g. phytoplankton community). The basic statistics in SEM are based on the associations between variables, as measured by as the covariance matrix ($\Sigma$). Estimating and evaluating the fit of SEM is done by comparing the model-implied covariance matrix (with model parameters $\theta$) and an observed covariance matrix, The null hypothesis is that $\Sigma = \Sigma(\theta)$.

For studying the phytoplankton dynamics in Lake Valkea-Kotinen and testing the value of SEM we first created a conceptual model of factors affecting phytoplankton abundance. Based on the observed correlations of the variables (IV) and previous knowledge the final conceptual model included the interrelationships between phytoplankton (chl-*a* as proxy), grazing zooplankton (*Copepods* and *Cladocerans*), nutrients (TP) and physical environment (water colour and water temperature). This model led to an expected covariance which was tested against the covariance matrix based on the observed data of Lake Valkea-Kotinen. The unknown parameters were estimated using the maximum likelihood (ML), generalized least squares (GLS) and asymptotically distribution free method (ADF) by minimizing the difference between the sample-based and model-induced covariances.

### 3.2.5 Bayesian inference for uncertainty analysis (III, IV, V)

The parameter estimation for the nutrient retention model and hierarchical model was done according to the Bayesian framework (III). The only unknown model parameter in the nutrient retention model was the settling velocity. No previous knowledge about the variation in the settling velocity was available, thus so-called non-informative prior distribution for the estimation was used. In cases like this, the prior is termed 'weak' or 'vague' and the posterior distribution is mostly influenced by the data (Zuur et al. 2009). The uncertainty in the nutrient retention model outcomes is formed by the parameter and residual error variances ($\tau^2$ and $\sigma_s^2$) and in the chl-*a* model by the model error variance ($\tau^2$).

SEM problems are often complex, and several parameters have to be estimated simultaneously. The Bayesian approach in SEM context makes specifying and solving these models more flexible (Gitzen *et al*. 2012) and allows for more precise estimation of the error terms. For the Lake Valkea-Kotinen case (IV), we used Bayesian theory especially for estimating the error distributions to obtain more realistic information about the variation in the errors concerning zooplankton ($\varepsilon_4$, $\varepsilon_5$) and TP ($\varepsilon_3$). These variance estimates were then used for constraining the error variances in the final SEM analysis. For the Bayesian analysis we used non-informative priors.

# 4 RESULTS

## 4.1 Performance of the wireless sensor network (I)

The wireless sensor network's performance was evaluated from the network maintainer's and data users' perspectives based on 1.5 years of experience. The required maintenance effort of the sensors depended on the measured parameters. The most laborious maintenance effort was the cleaning of the turbidity sensors because of the biofouling of the optical lenses. In total, these required cleaning on 64 occasions during the evaluation period (Table 3). Also, problems with the battery contact (40 occasions) and decreasing battery voltage (48 occasions) were reported. For weather parameters the rain gauges caused problems as they were clogged up 18 times. The weather stations also collapsed 12 times and there were other technical malfunctions 5 times. The abovementioned problems were manifested in the data as missing or suspicious values and they were detected with the automatic quality control tests (I, Chapter 3.2.1).

TABLE 3 Karjaanjoki wireless sensor network maintenance problems, how they occurred in the data and the intensity of the occasions during the evaluation period 6/2007−12/2008 (I).

| Problem | Manifestation in the data | Number of occasions |
|---|---|---|
| Turbidity sensor biofouling | Turbidity values increasing gradually | 64 |
| Decreasing battery voltage | Missing data and/or air humidity decreasing continuously | 48 |
| Problems with battery contact | Missing data | 40 |
| Organisms on the turbidity sensor | Saw tooth pattern in the data | several |
| Rain gauge clogged up | No accumulation of precipitation despite nearby rain | 18 |
| Station collapse | Possible problems with wind data and/or no precipitation | 12 |
| Station malfunction | Missing data or station down regardless of battery condition | 5 |

Based on the four months evaluation period, on average 0.6 % of the weather station data and 1.4 % of the turbidity data were missing due to battery problems. However, the amounts of missing data varied between sites and for one turbidity sensor over 10 % of the measurements were missing. Further, there were only three events where the measurements were outside of the predetermined error and warning limits (see Chapter 3.2.1). These were two exceptionally cold summer nights when the air temperature was less than the warning limit for the hemiboreal climatic zone of < 2 ˚C.

## 4.2 Uncertainty in the status class and monitoring (II)

The overall chl-*a* and TP metric mean uncertainty was estimated from the mixed effects model and expressed as the relative standard error of the mean (RSE %). The median total error was 10 % for the coastal chl-*a*, 6 % for the lake chl-*a* and 8 % for the river TP, varying considerably within the waterbody types (Fig. 4). In the individual lake waterbodies the chl-*a* uncertainty varied from 2 to 34% and in coastal waterbodies from 5 to 32%. The TP uncertainty in the individual river waterbodies varied from 2 to 44%.

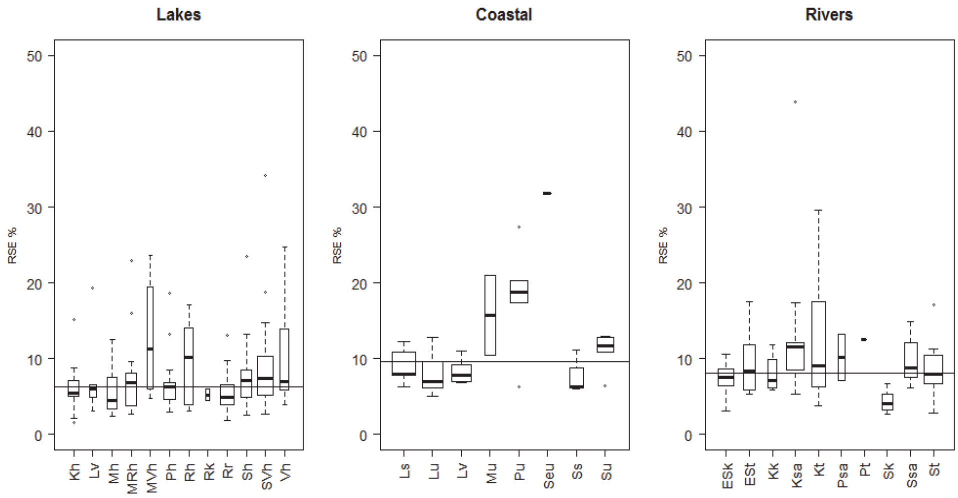


FIGURE 4 Total error (RSE %) of the mean metric for waterbody types for lakes, coastal areas and rivers. The box plots show the median, lower and upper quartiles and outliers. The box widths are proportional to the square roots of the number of observations in the water body type. The median RSE % of each water category is denoted as a vertical line (6 % for lakes and 10 % for the coastal chl-a, 8 % for river TP) (II).

For waterbodies with a single intensively monitored sampling site, the overall uncertainty was divided into temporal variances between years and months, and the residual variance that included all the unexplained variation. The residual variation was the most dominant in several waterbody types (Fig. 5). The annual variation was larger than the monthly variation for the coastal chl-*a*, and the other way around for the river TP. Between sampling site variation for waterbodies with more than one sampling site was the largest for lake chl-*a* within several lake types (see Fig. 5 in II).

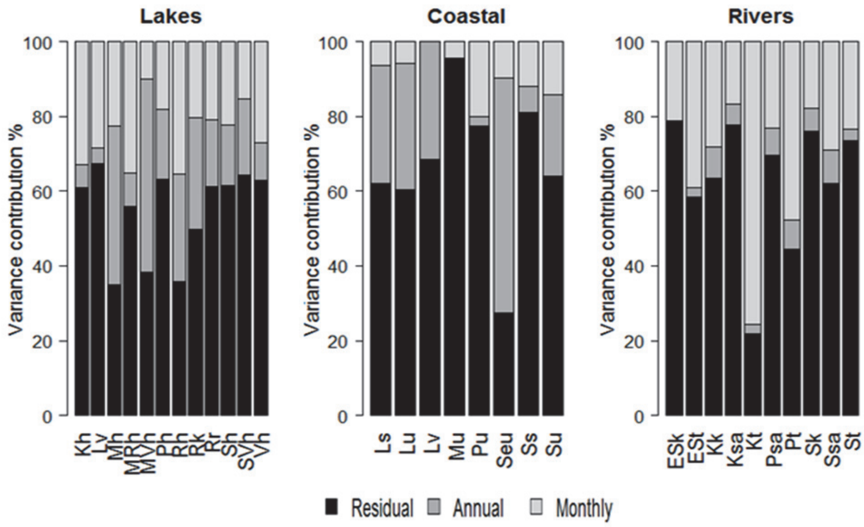


FIGURE 5 Percentages of temporal (annual, monthly) and residual variance components in chl-*a* status class uncertainty (lakes and coastal waterbodies) and TP (rivers) in different waterbody types (figure from II).

The confidence of the estimated status class was expressed as the probability of the most probable class. The confidence was generally high and the median probability of TP class within the river waterbodies was 96 %. For chl-*a* class within lake waterbodies the median probability was 83 % and within coastal waterbodies 88 %. However, the confidence of the class varied within the waterbody types (Fig. 6 in II) and between individual waterbodies. The lowest confidence of the status class was 43 % in lakes, 46 % in coastal waterbodies and 47 % in rivers.

The practical use for the uncertainty analysis was the statistical rules that can be used to support the decision making process when evaluating the efficiency of the monitoring and reallocating the sampling effort. For 108 (40 %) from the 272 intensively monitored waterbodies the sampling effort could have been reduced without losing the confidence of the status class. River TP mean estimate was usually precise and 63 % of the river waterbodies were sufficiently sampled for TP status classification. However, for chl-*a* the uncertainty was often high and, and based on the statistical rules, more sampling effort would be needed in almost 70 % of the intensively monitored coastal and lake waterbodies.

## 4.3 Nutrient loading response tool (III)

For increasing the precision of the chl-*a*-nutrient response a hierarchical Bayesian model was fitted (Chapter 3.2.2) to the large Finnish data set (Chapter 3.1.1). Based on the posterior distributions of the overall chl-*a* mean (fixed intercept), the overall TP, TN and their interaction (fixed slopes), the majority of the variation in the fixed effect is in the intercept, followed by the TP, TN and the interaction (III). There were substantial differences in the posterior distributions of the lake-type parameters. For example, the intercept of the large humic lakes showed larger positive chl-*a* differences compared to the overall mean of the other lake types.

The LLR model tool was tested for Lake Kuortaneenjärvi (III). The observed relationship between the in-lake TP concentrations and the TP loading are within the 90 % of the nutrient model prediction error (Fig. 5). The model parameter and residual error were separated in the models and from the total prediction uncertainty the proportion of the model residual error was greater than the model parameter error (Fig. 6).

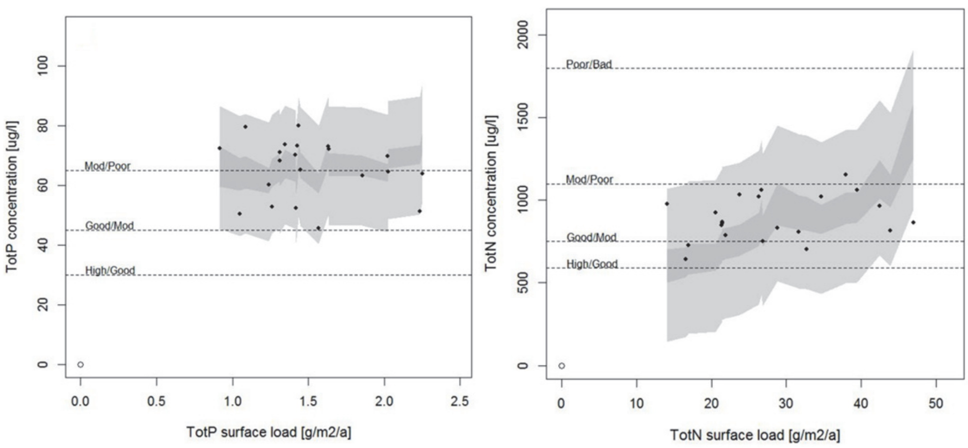


FIGURE 6 Model fit of the loading model for TP (on the left) and TN (on the right). The 90 % model parameter uncertainty is indicated in dark grey; the 90 % parameter uncertainty and residual error together are indicated in light grey. The observed values are shown as dots and horizontal dashed lines denote the status class limits (III).

Based on the modelled concentration probability distributions, the mean TP value of Lake Kuortaneenjärvi most probably indicates a Poor status class (51 %) and the TN indicates a Moderate status class (45 %). The status class probabilities of other classes are also considerable, 5–55 % for TP and 18–19 % for TN (Fig. 7).

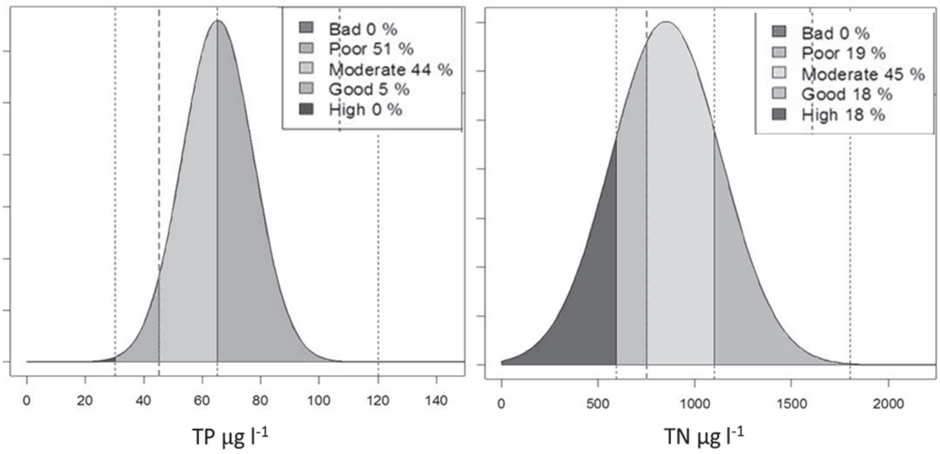


FIGURE 7 Predictive probability distributions of TP (on the left) and TN (on the right) concentrations with average TP and TN loadings for Kuortaneenjärvi. Different colours denote different status classes and the proportion of the colour denotes the probability with which the status is achieved (III).

According to the results, the phosphorus loading in Kuortaneenjärvi should be reduced by 30 % and the nitrogen loading by 13 % to achieve a Good nutrient status in the lake at 50 % confidence. On the other hand, with, e.g., 90 % confidence of exceeding the Good/Moderate TN class boundary the nitrogen loading reduction should be 60 %. The simultaneous effects of TP and TN loadings on the chl-*a* suggest a TP limitation of phytoplankton with low TP loadings and high TN loadings and a TN limitation with high TP and low TN loadings (Fig 7). Around the median chl-*a* concentration (25 µg $l^{-1}$), loading reductions made to both TP and TN would result in achieving the chl-*a* target G/M criteria of 20 µg $l^{-1}$. The chl-*a* model accounts for only the residual uncertainty and therefore the Moderate status class probability is 100 %. However, treating the nutrient model output as an input to the chl-*a* model introduces another source of uncertainty. Illustrating the effect of the nutrient model residual uncertainty on the chl-*a* prediction uncertainty the 25th and 75$^{th}$ percentiles from the simulated TP and TN distributions (Fig. 8) were calculated. The predictive chl-*a* distribution ends up wider and the confidence of the Moderate class is 73 % and confidence of Good, High and Poor classes 21 %, 4 % and 2 %, respectively.

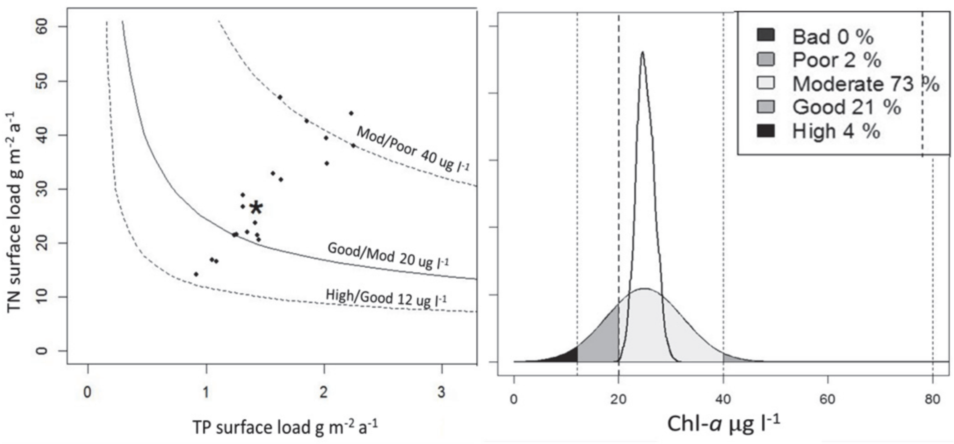


FIGURE 8 On the left: contours of chl-*a* showing the median chl-*a* estimate with different TP and TN loading combinations for Lake Kuortaneenjärvi. An asterisk indicates the median chl-*a* estimate with median nutrient loadings and dots indicate the observed loadings. On the right are the predictive probability distributions of chl-*a* concentrations when only the hierarchical chl-*a* model prediction uncertainty is accounted for (narrow bold line) and when the nutrient model parameters and residual uncertainty are accounted for. For the latter a different colour denotes the different status classes and the proportion of the colour denotes the probability with which the status is achieved (III).

## 4.4 Causal modelling of phytoplankton development (IV)

Structural equation modelling was tested to gain more insight into the phytoplankton development in the pristine small humic waters of Lake Valkea-Kotinen. The estimation methods (ML, GLS and ADF) used for the final SEM modelling gave similar results to the parameter estimates, and the ($\chi^2$) test statistic indicated a good model fit. The fit was further improved using the error parameters from the Bayesian uncertainty analysis ($\chi^2$ = 15.741, $df$ = 10, $p$ = 0.107). The Bayesian analysis indicated that the most dominant errors were attached to the biological parameter variance estimates, particularly copepods var($\varepsilon_5$). Based on the SEM results, the effects of the nutrients and water temperature on phytoplankton were positive and the effects of water colour and zooplankton grazing were weakly negative (Fig. 9 and Table 2 in IV). An initial correlation analysis indicated that the connection between water temperature and grazing was strong and this covariance could be accounted for and confirmed in SEM (0.86, $p < 0.001$, see also IV, Table 2). Copepods and Cladocerans describe the latent variable 'Grazing' relatively well as their loadings coefficients were high (0.61 and 0.83). TP did not fully represent the latent variable 'Nutrients' (0.56).

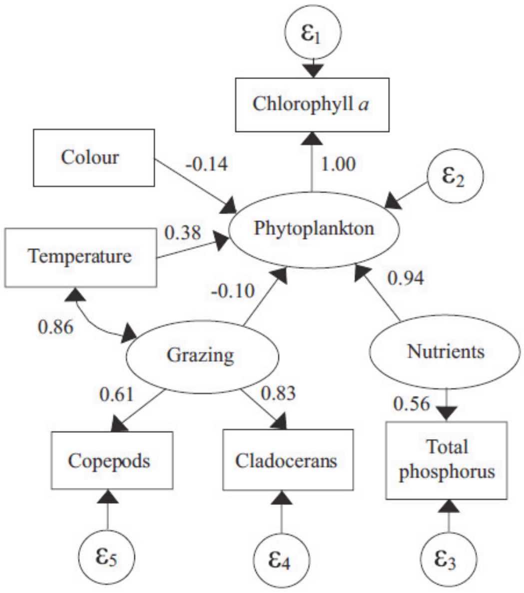


FIGURE 9 Structural equation model for Lake Valkea-Kotinen ($n$ = 144). The measured variables are indicated in rectangles, latent (unmeasured) variables in ovals, and error terms in circles. The arrows indicate the direction of effects, and 2-headed arrows indicate a correlation between variables. Numbers beside each arrow indicate the standardized path coefficient, or regression weights between the variables estimated using maximum likelihood (IV).

# 5 DISCUSSION

River basin management planning requires sufficient monitoring and suitable assessment tools for helping to estimate the status, loading responses and management impacts of water bodies. Environmental monitoring with wireless sensor networks produces large amounts of spatially and temporally representative data for multiple purposes (Hart and Martinez 2006, Hanson *et al.* 2016). These networks have been often evaluated by their technological challenges, such as communication and sensor failures (see, e.g., Akyildiz *et al.* 2008). However, there are also other aspects that result in problems with data quality as was shown in the case of Karjaanjoki river basin sensor network (I). Especially the field work effort, including calibration sampling, cleaning of turbidity sensors and rain gauges, were found to be laborious, costly and time-consuming (I). These findings do not differ from sensor networks studies especially related to water quality sensors as the performance of these networks relies strongly on regular maintenance activities and calibration data sampling (Xu *et al.* 2014, Pellerin *et al.* 2016). Ensuring good quality of any sensor produced data is highly important. Especially now that the costs of the sensors are falling and thus the amount of data and applications are increasing, there is a real need for automatic error diagnostics that alert maintenance needs in real-time (Thessler et al. 2011). If the data quality does not meet the end-user's requirements for data quality, there is a risk of the data being unused. Since deploying the Karjaanjoki sensor network, the water quality and weather data have been utilised, e.g., for determining more accurate suspended solids and phosphorus loads (Koskiaho *et al*. 2015), and soil moisture and weather data has been used for improving crop production processes at the farm level (Thessler *et al.* 2011). Despite the benefits gained with more accurate data, it has been difficult to find suitable long-term funding for maintaining such a large-scale sensor network. The current situation of the network is that 28 of the original 77 sensor nodes are still gathering data. To date, the sensors located at the Hovi wetland have been producing valuable data for the retention performance studies (Koskiaho *et al.* 2009, Linjama *et al.* 2009).

Monitoring programmes serving the WFD implementation and aiming at producing data for reliable status assessments should account, and ultimately aim to reduce the natural spatiotemporal variation of the biological and supporting (physico-chemical) quality elements (Carstensen and Lindegarth 2016, Cavallo *et al.* 2016). Using extensive data sets and mixed effects modelling we were able to estimate the chl-*a* or TP status class uncertainty for 278 Finnish waterbodies by distinguishing the variation between years, months and sampling sites (II). Our results suggested that the uncertainty, expressed as total error of the chl-*a* mean value was higher in coastal waterbodies than in lakes, which is in line with the fact that the coastal ecosystems are highly heterogeneous and the chl-*a* is usually highly variable (Kauppila 2007, Borja *et al*. 2013). Estimations of uncertainty stemming from several sources of variability has been seen as a central element related to ecological status assessment (Hering *et al*. 2010). For the lake chl-*a*, the year-to-year and between months variation seem to have a considerable influence on the classification uncertainty (Carvalho *et al.* 2013, Søndergaard *et al.* 2015). Based on a pan-European study, accounting for the spatial variation, it was shown that the within lake variability is smaller than between lake variation, which is in turn caused by eutrophication pressures and thus differences between TP levels (Thackeray *et al.* 2013). We were able to identify the most dominant sources of uncertainty and this information was used for developing practical decision-making rules for allocating the sampling effort so that overall metric uncertainty is reduced (II). The most dominant error source was the residual variability (II), which means that the overall variability could not be explained by yearly, monthly and sampling site variances. Even though we used the most intensively measured waterbodies, and were able to account for some of the spatiotemporal variation, the uncertainty assessments could be improved using other sources of data and fixed covariates in the model. For example, accounting for spatial (and temporal) variation with satellite data and for temporal variation with automatic sensor data would provide another scale and additional information to be used in the uncertainty analysis (Aplin *et al.* 2006, Anttila *et al.* 2012). In our study, the precision of the chl-*a* estimates were improved using national-scale data and hierarchical modelling accounting for the uncertainty at different levels (III).

When the precision of the status class metric is quantified, the uncertainty in the status classification can be assessed using probability distributions (II, III). However, when the ecological classification is expressed as probabilities there are different alternatives for setting the status class depending on how the probabilities are interpreted (Anon. 2003a). For example, the TN status class of Lake Kuortaneenjärvi (III) could be designated to three different status classes depending on which approach was applied. The fail-safe (/precautionary for the environment) approach designates the metric status to the ‘poor’ status class, because the probability of the class being better than ‘poor’ is less than 95 % (81 %), so it cannot be said with enough certainty that the status is better than ‘poor’. Following the benefit-of-the-doubt approach (precautionary for the polluter) leads to ‘good’ or ‘high’ status classifications, because the probability of not being in a worse class is less than 95 %. Based on the face-value approach the status becomes 'moderate' assessed as the mean value with 45 % confidence. The face-value approach is adopted in the Finnish assessment scheme (Aroviita *et al.* 2012, Andersen et al. 2016), thus disregarding the uncertainty of the classification and putting the burden of proof on both the polluter and the environment. However, the final ecological status class is not determined with one single metric value of one biological quality element (such as a chl-*a* metric for the phytoplankton quality element) but is constituted from multiple quality elements and multiple status class metrics (Anon. 2003a). Therefore, it is important to broaden the statistical uncertainty assessments to include other quality elements as well. This has been done for lake macrophytes (Dudley *et. al* 2013), river benthic diatoms (Kelly *et al.* 2009) and eelgrass shoot density in coastal environment (Balsby *et al.* 2013). In Finland and other Nordic countries, the lack of biological quality data complicates estimating the relevant sources of uncertainty.

When a waterbody suffering from eutrophication does not meet the ecological quality standards, the required nutrient loading reduction has to be evaluated. The LLR assessment tool (III) was developed for this purpose as it has the ability to combine external loading with the chl-*a* status. Even though such loading models, as in the LLR, are structurally and conceptually rather simple, the data and knowledge are often too limited for more complex ecosystem models or process-based mechanistic models (references in V, Shimoda and Arhonditsis 2015). Linking the empirical loading models to a statistical chl-*a* model seem to offer a promising tool assisting the management planning process. Hierarchical Bayesian modelling proved to be an efficient way to improve the chl-*a* predictions for a single lake using variation information from the national lake monitoring data (III, Malve 2007). Elsewhere, the hierarchical Bayesian approach has been taken with the nutrient loading modelling as well (Cheng *et al.* 2010). This would also be a significant improvement in development of the LLR as the clearest shortcoming of the LLR tool seemed to be the uncertainty related to the input loading data (III). This uncertainty could be reduced and thus the efficiency of management improved with more precise loading estimates and hierarchical structure of the nutrient modelling. However, these both require more and frequent lake-specific monitoring data, and automatic sensors, and sensor networks seem to provide a promising tool for this (I, Tattari *et al.* 2017).

Based on the LLR results, Lake Kuortaneenjärvi does not meet the water quality standards of its lake type (highly humic). Therefore, the lake would benefit from nutrient loading reductions and as a result the status should improve (III). However, for Lake Kuortaneenjärvi the management actions for reducing external loadings have been ineffective and the recovery from eutrophication seems to be very slow, especially because of the substantial internal loading (Hjerppe *et al.* 2017). In addition, even though the relationship between nutrient enrichment and eutrophication is well-studied and widely acknowledged in inland waters, little is known about the combined effects of diffuse pollution and other stressors such as climate change and morphological changes (Hering *et al.* 2015).

The multiple pressures and multiple water quality variables with varying sensitivity to different pressures make water management very complex, and variables are also often multi-correlated and measured with some degree of uncertainty. This was also the case in the study of phytoplankton dynamics in Lake Valkea-Kotinen (IV). In this case the suitability of structural equation modelling was tested, which ought to provide a way to investigate the relationships in a more flexible way between a set of correlated variables (Reckhow *et al.* 2005, Arhonditsis *et al.* 2006). Due to a lack of detailed biological data, our model was a simplified conceptualization of phytoplankton dynamics, and could address only limited study questions. On the other hand, using the data that is available efficiently for lake management is the purpose of implementing these statistical methods. The main result, that an increase in nutrients and water temperature have positive effects while colour and grazing have negative effect on phytoplankton, was in line with the results of earlier studies (Peltomaa *et al.* 2013, Arvola *et al.* 2014). However, the effect of grazing was more distinct with SEM than with traditional regression models. We were also able to gain new insights from the more detailed exploration of the interactions between phytoplankton and zooplankton. This information can support the long-term research and interpretation of results at Lake Valkea-Kotinen. Although the method has been used quite rarely in aquatic ecology so far (V), based on our experience with the Lake Valkea-Kotinen study, wider use of this statistical method is encouraged.

The statistical methods described in this thesis were chosen for many reasons. Multilevel and causal modelling frameworks (III, IV) are well suited for analysing sparse and heterogenic long-term monitoring data, and operating at varying spatial levels. Also, statistical evaluation of ongoing monitoring programmes (II) is necessary because the importance and efficacy of the monitoring under question. One benefit of statistical modelling over mechanistic modelling is that the former is faster to use for many waterbodies either consecutively or even simultaneously, and existing monitoring data is used efficiently (V). However, these data should be reliable and representative for different modelling purposes as well. Especially in Finland and other Nordic countries, for many water bodies the data on biological quality elements and supporting elements available for RBMP purposes are far from representative, or at present lacking completely (Andersen *et al.* 2016).

Statistical, data-based models are particularly useful for decision making under an adaptive management framework as they enable predictions to be made from the data and have measures of uncertainty associated with the outcomes (Anon. 2004). However, the definitions and expectations of adaptive management are complex and multidisciplinary. The term has been found hard to define explicitly and the framework is often challenging to implement in practice (Rist *et al.* 2012). There is a risk that adaptive management is only perceived as a “buzzword” and the actual systematic implementation remains abstract and loose. Therefore, all attempts to develop tools and methods for iteratively evaluating the causes and responses make the implementation of adaptive management more practical. It has also been pointed out that adaptive monitoring and management frameworks are considered successful if they provide the right data for the information needs in question, and the information is gained with the money that is available at the time (Loucks and van Beek 2005). The requirement of cost-efficiency is often a justifiable reason for evaluating ongoing monitoring programmes. However, it should be borne in mind that the costs of monitoring compared to the benefits gained through improved understanding are still very low (e.g., see the value of information of marine monitoring in Nygård *et al.* 2016).

# 6 CONCLUSIONS

Operating under the adaptive management framework requires continuous learning about the functioning of ecosystem, and methods that can adapt to the increased knowledge. Based on the results of this thesis, long-term monitoring and spatial-temporally dense sensor networks offer valuable information for better decision making in RBMP given that the data quality is assured, and suitable statistical methods are used for analysing the data. Although the studied statistical methods seem to offer a useful tool for dealing with uncertainty and support the decision-making process, they still are not fully utilized for WFD implementation in Finland. Efforts towards implementing these methods in practice are being pursued more actively. Therefore, based on the findings of this thesis, it is suggested that:

- The confidence (uncertainty) of the status classes should be statistically evaluated starting with the single metrics as was done here for chl-*a* and TP values. In order to gain broad and accurate uncertainty estimates of spatiotemporal variation, multiple data sources should be combined.

- Monitoring designs (frequency and coverage) should be systematically and iteratively evaluated with objectives that serve the RBMP

- Nutrient loading monitoring and modelling should be intensified especially for waterbodies whose external loading reductions are essential for improving their status. This can be partly done using automatic water quality sensors which are placed optimally.

- At least some simple statistical uncertainty estimate should be attached to any assessment tool to identify the information gaps and to inform decision making

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# YHTEENVETO (RÉSUMÉ IN FINNISH)

### Tilastollisia menetelmiä adaptiiviseen vesienhoidon suunnitteluun ja seurantaan

Yhteiskunnallinen huoli vesistöjen tilan heikentymisestä on kasvanut entisestään. Vesien tilaa ja sitä kautta niiden suojelua, hyödyntämistä ja virkistyskäyttöä uhkaavat erityisesti ihmisen toiminnan vaikutukset sekä ilmaston lämpenemisestä aiheutuvat muutokset. Vesistöjen suojelemiseen ja tilan parantamiseen tähtääviä toimia ohjataan lainsäädännöllä. EU:n vesipuitedirektiivin (VPD) tavoitteena on saavuttaa ja ylläpitää jäsenmaiden vesistöjen hyvä ekologinen ja kemiallinen tila. Kuuden vuoden välein tehtävissä vesienhoitosuunnitelmissa kuvataan vesistöalueittain vesien tila ja mahdolliset toimenpiteet tilan parantamiseksi. VPD:n toimeenpanon myötä ekologisesta tilasta ja tilaan vaikuttavista tekijöistä halutaan aikaisempaa kokonaisvaltaisempi kuva painottaen erityisesti biologisia tekijöitä sekä alueellista kattavuutta. Tämä on asettanut suuria haasteita vesistöjen seurantaan, tilanarviointiin ja hoitotoimenpiteiden suunnitteluun.

Käytännössä vesienhoitosuunnitelmien laatiminen on vaiheittainen prosessi, jossa vesistöjen seuranta tuottaa tietoa tilanarviointia varten, ja arvioidun tilan perusteella päätetään mahdollisista tilan parantamiseen tähtäävistä toimenpiteistä. Toteutettujen toimenpiteiden vaikutusten seurannalla saadaan edelleen uutta tietoa, jonka perusteella toimintatapoja voidaan muuttaa entistä tehokkaammiksi. Epävarmuutta päätöksentekoon aiheuttavat kuitenkin mm. toimenpiteiden vaikutusten arvioinnin vaikeus, aineistojen epäedustavuus, luonnollinen vaihtelu ja tilanarviointijärjestelmän monimutkaisuus. Vesienhoidon suunnittelun tuleekin olla adaptiivista, eli korjata seuranta- ja toimenpideohjelmia sitä mukaa kun saadaan uutta tietoa vesien tilasta ja toimenpiteiden vaikutuksista. Ympäristönseurannan resurssien jatkuva väheneminen sekä perinteisen vedenlaatuseurannan korvaaminen uusilla menetelmillä on lisännyt tarvetta kehittää arviointimenetelmiä, jotka hyödyntävät tehokkaasti seurannoista saatavaa tietoa ja huomioivat arviointeihin liittyvän epävarmuuden.

Tässä väitöstyössä on kehitetty ja testattu arviointityökaluja käytännön vesienhoidon suunnittelun tueksi. Tutkimuksessa on arvioitu eri tavoin tuotetun seurantatiedon luotettavuutta ja aineiston laatuun vaikuttavia tekijöitä. Työssä käytetyt tilastolliset menetelmät ottavat huomioon seuranta-aineistojen monitasoisen rakenteen, luonnossa esiintyvän ajallisen ja paikallisen vaihtelun sekä samalla tavoin ympäristöpaineeseen reagoivien vesi-muodostumien yhteiset tekijät. Menetelmät painottuvat erityisesti epävarmuuden arviointiin ja adaptiivisen vesienhoidon ja seurannan tarpeisiin.

Ympäristönseurannassa on otettu käyttöön perinteisen vesinäytteenoton lisäksi jatkuvatoimisia mittareita sekä useista mittauspaikoista muodostuvia sensoriverkkoja. Tässä työssä arvioitiin Karjaanjoen valuma-alueella edelleen osittain toimivan vedenlaadun, maankosteuden ja säämittausten verkoston toimintaa. Lisäksi arvioitiin automatisoidun mittausverkon pystyttämiseen, ylläpitoon ja laadunvarmistukseen liittyviä seikkoja erityisesti aineiston loppukäyttäjän näkökulmasta. Tällaisen sensoriverkoston on tuotettava luotettavaa ja käyttökelpoista aineistoa, jotta sitä voidaan käyttää hyödyksi erilaisissa ympäristötietoa käyttävissä sovelluskohteissa. Aineiston laadun tarkkailua varten kehitettiin automaattinen laadunvarmistusjärjestelmä hälyttämään epäilyttävistä tai puuttuvista mittaustuloksista ja sensoreiden huoltotarpeesta. Kehitetyn laadunvarmistusjärjestelmän avulla saatiin tietoa siitä, miten erilaiset sensorit toimivat ja kuinka paljon huoltotoimia tarvitaan laajan sensoriverkoston ylläpitoon. Karjaanjoen verkosto tuotti parhaimmillaan yli 10 miljoonaa mittauskertaa vuodessa, joista vain murto-osa oli ennalta määrättyjen mittauspaikkakohtaisten hälytysrajojen ulkopuolella. Eniten huoltotarvetta aiheuttivat vedenlaatumittareiden puhdistaminen ja mittausasemien virransaantiongelmat.

Havaintoaineiston laatu ja kattavuus ovat avainasemassa myös VPD:n toimeenpanoa palvelevassa pintavesien perusseurannassa, jonka tavoitteina ovat erityisesti ekologisen tilan ja tilassa tapahtuvien muutosten arviointi. Vesistöjen suuri määrä kuitenkin vaikeuttaa kattavien tila- ja vaikutusarvioiden tekemistä, eikä seurantamittauksia voida tehdä kaikista vesimuodostumista. Seurantaohjelmien tehokkuuden ja riittävyyden tilastollinen arviointi on välttämätöntä, kun halutaan sekä tuottaa tietoa kustannustehokkaasti että arvioida laskennallisen tilaluokan luotettavuutta. Väitöskirjan toisessa osatutkimuksessa arvioitiin luokittelun luotettavuutta, vaihtelun lähteitä, sekä erilaisten koeasetelmien ja näytteenottomäärien vaikutusta luokittelun varmuuteen. Työssä käytettiin laajaa, intensiivisesti mitattujen suomalaisten joki-, järvi- ja rannikkovesimuodostumien aineistoa. Lineaarinen sekamallinnus ja varianssikomponenttien määrittäminen mahdollistivat nykyisen seurantajärjestelmän tuottaman aineiston tehokkuuden ja erityisesti resurssien uudelleenkohdentamisen arvioinnin. Tulosten avulla pystyttiin tunnistamaan sekä ne vesimuodostumat, joiden seurantaa tulisi lisätä, mutta erityisesti myös ne, joiden mittauksia voisi vähentää tai kohdentaa aikaisempaa tehokkaammin.

Mikäli vesimuodostuma ei tila-arvion mukaan ole tavoitetilassaan, tilaa heikentävien kuormituslähteiden vaikutukset pitäisi pystyä mitoittamaan mahdollisimman tarkasti ja kustannustehokkaasti. Erityisesti rehevöitymisen vaikutusten arviointi on keskeisessä osassa vesienhoidon toimenpiteitä suunniteltaessa. Kolmannessa osatutkimuksessa kehitettiin mallinnustyökalu (Lake Load Response, LLR) ravinnekuormitusvaikutusten arviointiin. LLR-työkalun avulla voidaan arvioida ulkoisen ravinnekuormituksen vaikutus järven kokonaisravinteiden ja kasviplanktonin määrään sekä todennäköi-syyksiin saavuttaa tavoitetila. LLR on jo osoittautunut hyödylliseksi käytännön vesienhoitotyössä, koska se mahdollistaa kuormitusvähennystarpeen laskemisen useille vesimuodostumille nopeasti ja melko suppeilla lähtötiedoilla. LLR-työkalun mallinnus perustuu yksinkertaisiin yhteyksiin vedenlaadun ja kuormituksen välillä. Mallinnuksessa hyödynnetään hyvin laajaa suomalaisten järvien havaintoaineistoa sekä hierarkkista mallinnusta, jonka avulla pystytään erittelemään epävarmuudet mallin rakenteessa ja havaintoaineistossa. Mallityökalun käyttöä testattiin Kuortaneenjärvelle, joka kärsii rehevöitymisestä, eikä ole saavuttanut tavoitetilaa hoitotoimenpiteistä huolimatta. Tulosten perusteella Kuortaneejärven ulkoisen kuormituksen vähennysten tulisikin olla merkittäviä, jotta hyvään tilaan päästäisiin.

Rakenteeltaan yksinkertaiset tilastolliset mallit ovat tehokkaita, kun halutaan saada nopeasti tietoa useasta eri vesimuodostumasta ja esimerkiksi niiden kuormitusvähennystarpeesta. Vesien tilaan vaikuttavat tekijät ovat kuitenkin hyvin monimutkaisesti sidoksissa toisiinsa ja syy-seuraussuhteet ovat usein epäselviä. Neljännessä osatutkimuksessa testattiin tilastollista rakenneyhtälömallinnusta arvioitaessa kasviplanktonin esiintymiseen vaikuttavien tekijöiden keskinäisiä suhteita. Tulosten perusteella saatiin lisätietoa mm. vesien tummumiseen liittyvän tutkimuksen tueksi, mutta ennen kaikkea kokemusta rakenneyhtälömallien soveltuvuudesta vesienhoidon suunnittelun tarpeisiin. Erityisen hyödylliseksi tämän lähestymistavan teki se, että toisin kuin useissa perinteisemmissä lähestymistavoissa, rakenneyhtälömallissa otetaan mittausvirhe huomioon ja selittävien tekijöiden välinen korreloituneisuus on sallittua.

Kaiken kaikkiaan tässä työssä esitellyillä tilastollisilla menetelmillä pystyttiin tuottamaan aikaisempaa tarkempia ennusteita vesien tilasta ja kuormitusvaikutuksista. Kaikissa näissä arvioinneissa on otettu huomioon epävarmuus, joka on väistämättä merkittävää, koska seurantatiedoissa on puutteita, toimenpiteiden vaikutukset vesistöihin on hankala arvioida ja arviointimallien rakenteita on välttämätöntä yksinkertaistaa. Tulosten mukaan epävarmuus johtuu hyvin usein mallinnuksen kannalta riittämättömistä syöttötiedoista tai huonosti allokoiduista seurannasta. Vaikka käytetyt tilastolliset menetelmät soveltuvat ekologisille muuttujille yleisemminkin, tässä työssä havaintoaineistona on käytetty yksinkertaisia vedenlaatua kuvaavia muuttujia (kokonaisravinteet ja a-klorofylli) nimenomaan biologisten aineistojen vähyyden vuoksi. Tehokkaan vesienhoidon kannalta sekä biologisia muuttujia että vesistöjen ravinnetaseita tulisi mitata entistä kattavammin.

Toimiminen adaptiivisen vesienhoidon edellyttämällä tavalla vaatii jatkuvaa oppimista ekosysteemien toiminnasta sekä menetelmiä, jotka pystyvät huomioimaan tiedon päivittymisen ja epävarmuuden päätöksenteossa. Tämän väitöstyön tulokset osoittavat, että sopivien tilastollisten mallinnusmenetelmien avulla laajoista seuranta-aineistoista saadaan tuotettua arvokasta tietoa vesienhoidon tueksi myös yksittäisen vesimuodostuman tasolla. Vaikka työssä käytetyt tilastolliset menetelmät vaikuttavat lupaavilta erityisesti epävarmuuden arvioinnissa, niiden käyttö on ollut suhteellisen vähäistä käytännön vesienhoidon suunnittelussa. Tutkimuksen perusteella voidaan ehdottaa, että jatkossa seurantaohjelmien tilastollista edustavuutta ja tarkkuutta, sekä tuotetun tiedon epävarmuutta pitäisi arvioida entistä systemaattisemmin, ja ennen kaikkea hyödyntää tätä tietoa seurantojen, ja tilanarvioinnin ja hoitotoimenpiteiden kehittämisessä. Lisäksi vesienhoidon suunnittelun tueksi kehitettyihin mallinnustyökaluihin tulisi liittää epävarmuusarvio, joka osaltaan auttaisi arvioimaan puutteet tiedontuotannossa, sekä epävarmuudet ja riskit hoitotoimenpiteiden vaikutuksissa.

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# ORIGINAL PAPERS

# I

## WIRELESS IN-SITU SENSOR NETWORK FOR AGRICULTURE AND WATER MONITORING ON A RIVER BASIN SCALE IN SOUTHERN FINLAND: EVALUATION FROM A DATA USER'S PERSPECTIVE

by

Niina Kotamäki, Sirpa Thessler, Jari Koskiaho, Asko O. Hannukkala, Hanna Huitu, Timo Huttula, Jukka Havento & Markku Järvenpää 2009

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*Article*

# Wireless *in-situ* Sensor Network for Agriculture and Water Monitoring on a River Basin Scale in Southern Finland: Evaluation from a Data User's Perspective

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**Abstract:** Sensor networks are increasingly being implemented for environmental monitoring and agriculture to provide spatially accurate and continuous environmental information and (near) real-time applications. These networks provide a large amount of data which poses challenges for ensuring data quality and extracting relevant information. In the present paper we describe a river basin scale wireless sensor network for agriculture and water monitoring. The network, called SoilWeather, is unique and the first of this type in Finland. The performance of the network is assessed from the user and maintainer perspectives, concentrating on data quality, network maintenance and applications. The results showed that the SoilWeather network has been functioning in a relatively reliable way, but also that the maintenance and data quality assurance by automatic algorithms and calibration samples requires a lot of effort, especially in continuous water monitoring over large areas. We see great benefits on sensor networks enabling continuous, real-time monitoring, while data quality control and maintenance efforts highlight the need for tight collaboration between sensor and sensor network owners to decrease costs and increase the quality of the sensor data in large scale applications.

**Keywords:** Sensor networks, agriculture, environmental monitoring, data quality, network maintenance.

## 1. Introduction

The rapid development of sensor and wireless communication technologies has increased the use of automatic (wireless) sensors in environmental monitoring and agriculture [1]. The availability of smarter, smaller and inexpensive sensors measuring a wider range of environmental parameters has enabled continuous-timed monitoring of environment and real-time applications [2,3]. This was not possible earlier, when monitoring was based on water sample collection and laboratory analyses or on automatic sensors wired to field loggers requiring manual data downloading. During the previous decades, environmental monitoring has developed from off-line sensors to real-time, operational sensor networks [4] and to open Sensor Webs. These are based on open, standard protocols, interfaces and web services [5-7].

Varying terminology, such as wireless sensor networks, environmental sensors networks [4] and geo-sensor networks [8], are used interchangeably to describe more or less the same basic concept of collecting, storing and sharing sensor data, but employing different technologies or having different functional focus [2]. All of these terms refer to a system comprised of a set of sensor nodes and a communication system that allows automatic data collection and sharing through internet based databases and services [2,4]. The sensor webs are also seen as an advanced part of sensor networks by some authors [4,8], while others differentiate between sensor networks and sensor webs. They emphasize that the latter are based on open Sensor Web enablement (SWE) standards and web services, and that sensor nodes are able to communicate with each other. This makes sensor webs interoperable and intelligent systems that can react to changing environmental conditions [2,5,6].

Along with developments in sensor and communication technology, complex environmental problems such as eutrophication and climate change have rapidly increased the need for temporally and spatially accurate data [4]. Adaptation to more variable weather and environmental conditions increases the importance of (near) real-time information that is valuable in better timing and control of agricultural management practices such as irrigation and pesticide spraying, monitoring algae bloom, and developing flood and frost warning systems [1,3]. The agricultural and food sector has also faced growing demands for traceability and quality of products in terms of environmental impacts of food production and food safety. This means optimizing cultivation inputs so that high yields are obtained and environmental effects are minimized. Several multinational and national initiatives aiming to improve quality of sea, lake and river water need more accurate information on effective means to decrease contaminants and nutrient discharges to waters and lower their effects, such as cyanobacteria blooms [9-11].

In order to function properly, sensor networks for water monitoring and agriculture normally require a relatively dense deployment of sensors. This leads to applications that monitor mostly local weather and soil characteristics [4]. Agricultural sensor networks have been developed for frost [3] or crop pest warning [12]. They are also an essential component in more advanced decision support systems (DSS) for crop protection [13,14]. In precision agriculture the studies have been concentrated on spatial data collection through mobile, vehicle embedded sensors or *in-situ* sensors deployed in the field [1]. Precision irrigation and fertilization and husbandry monitoring systems based on sensor networks have also been developed [1,15]. In water monitoring sensor networks are used for monitoring water quality and hydrology of rivers, lakes and reservoirs and for flood warning [4,5,16-19].

Although sensor networks still struggle with technical problems, such as energy-consumption, unreliability of network access and standard or software mismatches [20- 22], they have already been used for long-term monitoring under harsh outdoor conditions. They allow monitoring remote, hazardous, dangerous or unwired areas, for instance in the monitoring and warning systems for tsunamis, volcanoes, or seismologic phenomena. The sensor webs, in turn, are an emerging technology, that is not yet in operational use outside the test beds [6].

The sensor networks and sensor webs have a profound effect on the collection and analysis of environmental data. The data is very heterogeneous and may come from different *in-situ*, mobile or satellite sensors that have different temporal and spatial resolutions that may vary in accuracy and content [8]. Furthermore, the user has less control over data quality, and information needs to be extracted from a large amount of heterogeneous data. This highlights the importance of comprehensive metadata describing the sensors, data, and data quality, as well as the need for effective tools for data mining or other data gathering [4].

We present here a wireless sensor network (WSN), called SoilWeather, which aims to provide temporally and spatially accurate information, data services and (real-time) applications for water monitoring and agriculture on river basin and farm scales. We evaluate the performance of the network from the data user and network maintainer perspectives, and thus, focus on maintenance and data quality issues as well as applications. The technological development, solutions and standards are already comprehensively discussed in review articles of Yick *et al*. [21] and Akyildiz *et al*. [22]. We also discuss the challenges facing the SoilWeather WSN and the opportunities it has provided. Finally we conclude with the lessons learned from deployment and 1.5 years of running of network.

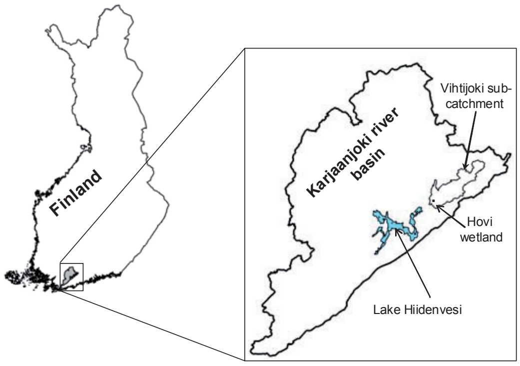
## 2. SoilWeather sensor network and applications

### *2.1. Karjaanjoki river basin*

SoilWeather is an operational river basin scale *in-situ* wireless sensor network that provides spatially accurate, near real-time information on weather conditions, soil moisture and water quality with a high temporal resolution all-year round. The network was established in Southern Finland during the years 2007 and 2008 and it covers the entire 2,000 $km^2$ Karjaanjoki river basin which is located in south west Finland (Figure 1). The catchment is mainly covered by forest (63%) and agricultural areas (17.7%). In the north part of the area the River Vanjoki and River Vihtijoki bring waters to Lake Hiidenvesi (area 29 $km^2$, mean depth 6.7 m) from which waters flow via River

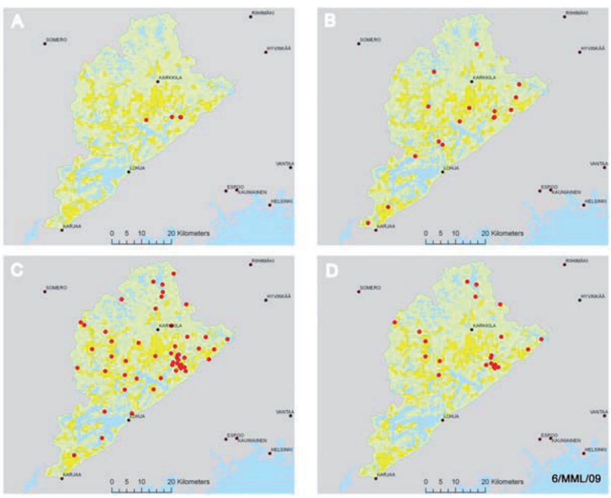
Väänteenjoki to Lake Lohjanjärvi (area 92 $km^2$, mean depth 12.7 m). Finally, the Mustionjoki river transports water from the river basin to the Gulf of Finland. In the northern parts of the river basin geology is dominated by quartz and feldspar. In the south the bedrock is granite. The soil is mainly clay, silt and glacial till [23].

**Figure 1.** Location of the Karjaanjoki river basin in Finland and the intensive measuring areas of Lake Hiidenvesi, the Hovi farm and the Vihtijoki sub-catchment.




The weather stations are evenly distributed around the catchment (Figure 2). They serve the purposes of catchment wide run off modeling. The turbidity and soil moisture sensors are scattered around the catchment as well, still majority of them are placed on the areas of different applications, which are explained later. Specific nutrient measurement stations are placed totally on the local application areas.

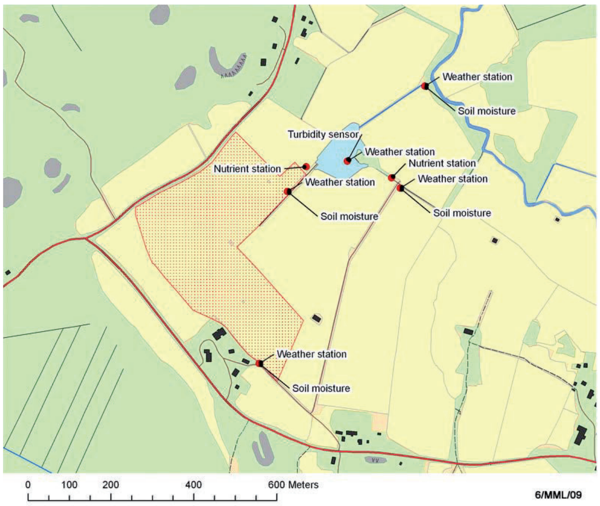
**Figure 2.** The location of the different SoilWeather WSN stations and sensors in the Karjaanjoki river basin. (a) Nutrient measurement stations. (b) Water turbidity sensors. (c) Weather stations. (d) Soil moisture sensors.



There are three intensively measured areas within the river basin: Hovi farm, Vihtijoki sub-catchment and Lake Hiidenvesi (Figure 1). The sensors are mainly located on land owned by private farmers, who are also the main users of the data. Eleven of the weather stations are placed in or close to potato crops for potato late blight warning. In addition data from one weather station close to a potato late blight control experiment at Jokioinen outside the SoilWeather network was used to evaluate the validity of potato late blight forecasts. The water measurements are obtained mainly in the rivers, but also in relatively small ditches and in constructed wetland within the Hovi intensive measurement area.

In the Hovi farm (25 ha) we measured soil moisture, weather and water quality at a field parcel level. The Hovi farm in Vakola is owned by the governmental MTT Agrifood Research Finland research institute. The soils are mainly clay, silt and glacial till and altitudinal variation is low (up to 130 m). Crops include barley, grass, turnip rape and wheat. Constructed wetland was built at Hovi farm in 1998 for water treatment, biodiversity and landscape purposes. The catchment of the wetland (12 ha) is under cultivation. It is a relatively large constructed wetland, ca. 5 % of the whole catchment [24]. One turbidity sensor is installed in the middle of the wetland and two spectrometers measuring nutrient concentration are located in the inflow ditch and close to the mouth of the outflow ditch of the constructed wetland to monitor its effectiveness in nutrient retention. Additionally, there are five weather stations in the area of the Hovi farm. (Figure 3).The spatially dense instrumentation of Hovi enables monitoring and testing of water protection methods and management practises and studying nutrient leaching from agricultural land in varying weather conditions at the field parcel level.

**Figure 3.** The locations of the SoilWeather WSN's weather stations, soil moisture sensors, nutrient stations and turbidity sensors in the area of Hovi farm.




The Vihtijoki sub-catchment, located in the north-west of the Karjaanjoki river basin, is instrumented with 25 weather stations and six water turbidity sensors. The turbidity sensors are located in the upper, middle and lower parts of River Vihtijoki to obtain validation data for the modelling efforts on transport of phosphorus (P) and total suspended solids (TSS) at a catchment level. Here, the SWAT (Soil and Water Assessment Tool) model will be used. SWAT is a catchment-scale model that operates on a daily time step [25, 26] and simulates water and nutrient cycles. SWAT model needs time series of many weather parameters as a part of input data. We intend to test the sensitivity of the model to the frequency of weather stations, i.e. if, and how much, will the results improve when the number of the weather stations will be increased in the model-setup, which will be established in the Vihtijoki sub-catchment (Figure 1).

Lake Hiidenvesi is one of the largest lakes in Southern Finland. It has recreational importance and it serves as a backup drinking water reserve for the inhabitants of the Finnish capital area. Restoration of the lake was started already in 1995 due to low water quality but improvements in water quality have not been gained so far [41]. The SoilWeather WSN has been used to monitor the water quality of the inflow and outflow of the lake using two nutrient measurement stations and one turbidity sensor.

*2.2. Sensors, sensor network and infrastructure*

The Soil Weather WSN hosts 70 sensor nodes altogether; 55 compact weather stations, four nutrient measurement stations, and 11 turbidity measurement stations. Six of the turbidity stations have water level pressure sensors as well. The typical setup of a weather station includes a weather station core and sensors for air temperature, air humidity, precipitation, wind speed and wind direction. Connected to the weather station cores there are also sensors for soil moisture and for water turbidity so that the network observes in its entirety soil moisture in 30 sites, turbidity in 18 sites and water level in eight sites.

**Table 1.** The sensors used and the parameters measured in the SoilWeather WSN.

| Sensor node | Sensors | Parameters | Producer's web page |
|---|---|---|---|
| a-Weather station basic core | Pt1000 | Temperature | www.a-lab.fi |
| | AST2 Vaisala HMP50 | Humidity | www.vaisala.com |
| | Davis Rain Collector II | Precipitation | www.davisnet.com |
| | Davis Anemometer | Wind direction | |
| | Davis Anemometer | Wind speed | |
| Additional parameters | Decagon ECHO (capacitance) | Soil moisture | www.decagon.com |
| | FDR (Frequency Domain Reflectometry) | Soil moisture | www.a-lab.fi |
| | OBS3+ | Water turbidity | www.d-a-instruments.com/ |
| | Keller 0.25 bar | Water level | www.keller-druck.ch |
| Nutrient measurement station | s::can spectrometer | Nitrate conc. | www.s-can.at/ |
| | | Water turbidity | |
| | | Water level | |
| | | Water temperature | |

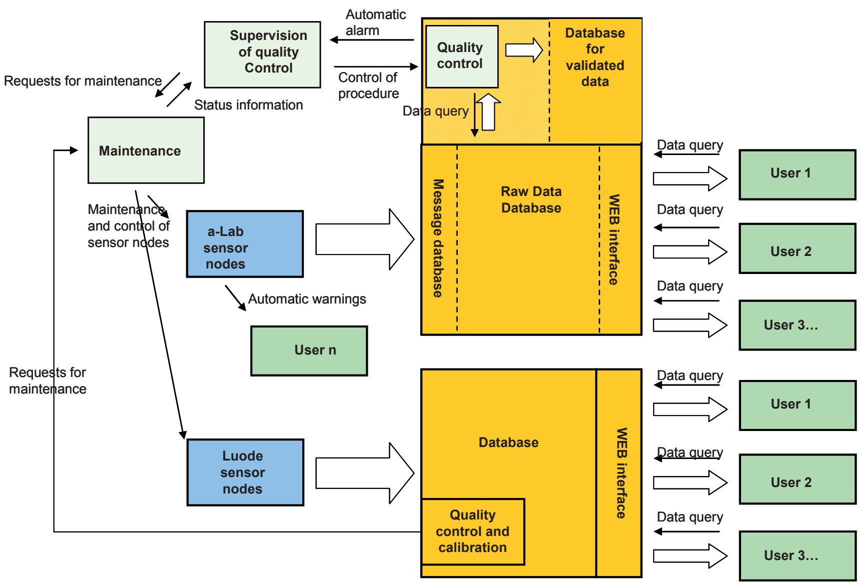
Nutrient measurement stations measure water turbidity and nitrate concentration with spectrometers employing ultraviolet and visible (UV-Vis) wavelengths. The setup includes also sensors for water level and temperature. All the sensor nodes have been geo-located in the field using a hand-held GPS device Trimble GeoXT. The sensor nodes, sensors and parameters measured are shown in Table 1.

SoilWeather WSN uses off-the-shelf sensors, nodes and server services provided by various sensor vendors. Each sensor node has a central processing unit with a GSM modem and SIM-card installed either into a weather station core or into a nutrient measurement station. The weather station cores can be controlled remotely by SMS messages or locally by connecting sensor nodes to the computer. The cores can also be programmed to produce automatic SMS alerts e.g. on drought, frost or moisture conditions predisposing to plant diseases.

The network uses time-based data collection. The frequency for nutrient measurements is once every hour, all the other sensors measure once every 15 min. Each sensor node collects and transmits the data independently to the database server, either as a SMS message (a-Weather station cores) or as a data call (nutrient measurement stations). The weather station cores are wireless and automatic; GSM and GPRS techniques are used in the data transfer and storing. GSM modems receive SMS messages, GPRS messages are transferred through HTTP interface. These messages are written to a message database and decoded with a parser program to measurements and timestamps. This information is then written to the final database.

The near real-time data is available as graphs and downloadable tables in two different internet-based data services provided by the sensor vendors. One of the services also supports XML-based data transfer. Diagram of the data flow in SoilWeather WSN is presented in Figure 4.

**Figure 4.** The data flow (white arrows) and communication system with main data services of SoilWeather WSN. a-Lab sensor nodes refer to nodes employing a-Weather station cores, Luode sensor nodes refer to nutrient measuring stations.



The SoilWeather WSN functions all-year round. Due to freezing of the sensors, measurements are less accurate in cold winter times, as there is no heating in the rain gauges or wind sensors. Also, the sensors located in rivers may be temporally removed during winter, as moving ice might break the sensor probes.

The weather stations are compact devices including all the sensors installed and they are easy to deploy. The weather stations are programmed to connect to the server automatically. For water turbidity and nutrient measurements, the easiness of deployment is very much dependent on environmental conditions, such as the ground material of the river bank and river bed, the river run-off, and existence of constructions. The sensor nodes are transferring data independently, and network is flexible to some extent; it does not demand reprogramming or updating of the existing nodes when new node or sensor is added. The sensor nodes use a battery package of two 6 V batteries.

At the moment, the data for the whole network is available only for participants of the project. The weather measurements are, however, freely available for the previous month through the open interface at the web site http://maasaa.a-log.net/ (in Finnish) and through the web site of Helsinki Testbed (http://testbed.fmi.fi/) after registration to researcher's interface.

### *2.3. Data quality control and network maintenance*

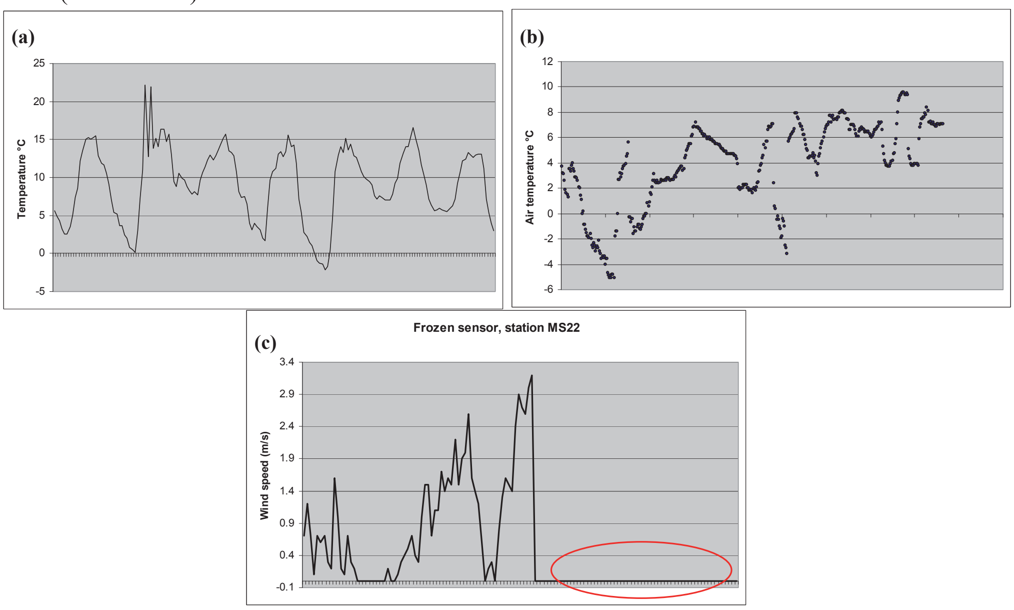
We see data quality as a broad concept including aspects of deployment, maintenance, cleaning, calibration and automatic data quality control algorithms. Careful deployment of sensor probes is the basis for ensuring good data quality. The location of the probe should be representative, considering the parameter measured. Weather stations are located in open and relatively flat areas and water turbidity sensors in the main run-off in location with no nearby discharging ditches or tributaries. The probes are mainly deployed by the same experienced field assistants from nearby MTT Vakola farm and by following sensor specific procedure. However, the final location of the sensor probes was always decided by the application, and negotiations with the land owners. The probes are also located so that they do not hamper cultivation practices or the recreational use of the river.

All the water and soil sensors are calibrated against water or soil samples, respectively. For weather stations no calibration in the field is done. Calibration samples for water measurements are taken once a month to ensure the quality of the sensor measurements and the correct functioning of the sensors. River discharges are available close to the location of the water measurements. Soil moisture calibration samples were taken soon after the deployment.

Reliable functioning of the sensors requires maintenance often enough. We maintain sensors on a regular basis, twice a year, but also occasionally when additional maintenance is needed. The maintenance procedure is sensor type specific. For weather stations the batteries are changed once a year, the fixation of instruments is checked and fixed if needed, and the equipment is cleaned. The water turbidity sensors and nutrient measurement stations need extra care because the optical lenses get contaminated in the water. The spectrometers are cleaned automatically with air-pressure and in addition manually once a month. Some of the water turbidity sensors are equipped with automatic wipers. The wipers were not available during the first deployments so the sensors were manually cleaned in regular basis: in winter time every month and in summer time when needed, approximately once a week.

Automatic data quality control system, that warns when suspicious data is received, was developed during the project to notify on maintenance needs. Different kinds of data quality problems that can occur in the SoilWeather WSN data are shown in Figure 5. In the first chart (a) there are two suspicious spikes in the temperature data. Rather common situation of missing data is shown in the second chart (b) and in the third chart (c) the wind speed is for some reason measuring the same value (0 m/s) all the time. In the beginning of the project there were only a few stations providing data to be checked and the quality control was carried out manually. As the amount of stations, and therefore the amount of the data, grew, it was essential to develop an automatic quality control and warning system. At the moment the system checks the data from all the a-Lab sensor nodes. For the four nutrient measurement stations Luode Consulting handles the quality control manually using their strong expertise and experience in this field.

**Figure 5.** Problems that have occurred in SoilWeather WSN data. Y-axis denotes different parameters and the x-axis denotes time (approx. 1 week). (a) Suspicious spike in air temperature data. (b) Gaps in the air temperature data. (c) Wind speed is constantly 0 m/s (no variation).




The automatic quality control runs under the UNIX system. The computer of the data quality controller logs in to the a-Lab server via SSH tunnel and retrieves data using Matlab Database Toolbox. . After the tests are run in Matlab, the quality controlled data is returned to a new database in a-Lab server. At the moment there are four different tests running in near real-time:

1) missing data test
2) missing observations test
3) variation test and
4) range test.

The missing data test checks if the data has been sent correctly. If no observations have come from the sensor within the period after the last check, the system saves an error report. Meanwhile the missing data test checks long periods of missing data, the second test searches for occasional missing values. The third test is for checking if the measurements vary over time. Presumably there is something wrong with the station or the sensor if the sensor measures the same value consistently (for 24 hours in this case). Finally, the range test tests if the measurement lies between predetermined range values. For meteorological parameters limit values were configured based on seasonal climate extremes and limit values vary according to the month and the climatic zone. The climatic zone of the Karjaanjoki river basin is hemiboreal and the range values in this case for air temperature are shown in Table 2. Limit values for meteorological parameters are provided by the Finnish Meteorological Institute (FMI). Soil humidity, turbidity and water level ranges are defined for every sensor separately, depending on the characteristics of soil, riverbed and river hydrology. For every observation the system gives an information label (flag) that indicates the quality level of the observation according to the range test. The flag value indicates whether the observation is correct (between the range values), suspicious (differs slightly from the range value) or wrong (differs dramatically from the range value). The range test and the flagging follows the system used in FMI [28].

**Table 2.** The monthly range limits (ºC) for air temperature in hemiboreal climatic zone. Warning_low and warning_high denotes the range limits for suspicious values, error_low and error_high the range limits for meteorologically impossible values.

| MONTH | WARNING_LOW | WARNING_HIGH | ERROR_LOW | ERROR_HIGH |
|---|---|---|---|---|
| 1 | -37 | 11 | -47 | 17 |
| 2 | -35 | 11 | -45 | 17 |
| 3 | -31 | 15 | -41 | 22 |
| 4 | -19 | 23 | -29 | 27 |
| 5 | -7 | 29 | -17 | 31 |
| 6 | -2 | 32 | -12 | 36 |
| 7 | 2 | 33 | -8 | 36 |
| 8 | 0 | 32 | -10 | 36 |
| 9 | -7 | 26 | -17 | 31 |
| 10 | -16 | 19 | -26 | 28 |
| 11 | -23 | 12 | -33 | 20 |
| 12 | -35 | 10 | -45 | 16 |

All the error messages from the past 24 hours are collected and sent automatically by e-mail to the data controller every morning. After the notification, the controller checks the data manually and makes the decision weather to inform the maintenance team or not. All the maintenance and the cleaning activities are stored in the log file of the sensor node and the log file is available for users through the data services.

### *2.4. Applications*

SoilWeather WSN is designed to be a multi-functional network. During the two-year pilot project, it has been utilised in the following applications:

- in predicting potato late blight risk
- in developing interpolation methods for weather parameters into 30 m resolution grid
- in monitoring water quality and nutrient retention in rivers and in constructed wetland
- in improving hydrological model at river basin scale
- in leaching model in sub-catchment scale
- in soil moisture model at field parcel level
- in precision agriculture.

It has also been used to study the relationship between local weather conditions and nutrient leaching. The network enables monitoring weather-related phenomena, such as heavy rains and the nutrient load peaks they induce. The SoilWeather WSN is used in research and in governmental monitoring tasks, but also by private farmers, who can use local data in planning and executing management practices. Here we present and analyze two applications in detail: predicting potato late blight risk in the farms, and the monitoring of constructed wetland.

Potato late blight caused by an oomycete, *Phytophthora infestans*, is one of the most devastating potato diseases worldwide. The potato crop can be completely destroyed within a few days if the weather is conducive for disease progress (Figure 6). In modern conventional potato production late blight can be effectively controlled with a range of chemical fungicides. The potato crop must be protected from emergence to harvest for each single day when weather enables late blight infection. Fungicide applications are necessary at 3 – 10 days intervals throughout the growing season resulting in 4 – 10 consecutive sprays in Nordic production and more than 20 sprays in the most intensive potato production regions in Western Europe [29, 30].

**Figure 6.** Potato late blight can totally destroy potato crop. Consecutive fungicide applications (green area in the front) are needed for effective control of blight. (Photo: MTT.)

To optimize the number of fungicide applications per season numerous weather based blight forecast models have been developed since the 1950s [31]. In the Nordic countries a late blight forecast model (NegFry) developed by Fry *et al*. [32] has been widely used since the 1990s [13]. Dramatic changes in the epidemiology of potato late blight pathogen have made the old NegFry model unreliable in certain occasions [33, 31]. Therefore a more recent potato late blight model (LB2004) introduced by Andrade-Piedra *et al.* [34] has been modified for use in the Nordic climate [35]. The characteristics of current Nordic potato late blight populations for the model development were studied in detail [36] and essential epidemiological parameters needed in the model were updated [37]. Sub-model calculation periods when the temperature is over 8 °C and relative humidity is over 90 % [35] was used to predict blight risk in this study.

The blight risk was calculated for the 11 weather stations at the potato fields and at the weather station at late blight control experiment at Jokioinen. The potato fields were visited twice a week from the last week of June to the first week of August. The occurrence of potato late blight was recorded and the onsets of blight epidemics were reported in the Web-Blight warning service (www.web-blight.net). The severity of blight as a percentage of defoliated leaf area was assessed at the experiment at Jokioinen three times a week.

Constructed wetland studies were made during 1999–2002 at the previously mentioned Hovi wetland [24]. As for the monitoring of water quality of inflow and outflow, the measurements were based on water sampling. Although the sampling earlier was flow-proportional and rather frequent, most of the days were left unmonitored. However, these days may include short-termed peaks of high runoff, which remain unknown. Typically, the gaps between the sampling days have been filled by e.g. linear interpolation, but the loading estimates tend to be more or less erroneous. Flow variations and thus also the error is particularly significant in small, agricultural, high-sloped catchments like the Hovi farm. For this defect, automatic sensors providing non-interrupted data offer a revolutionary improvement. To test this new monitoring approach in wetland research, s::can -sensors (Table 1) were installed in October 2007 for monitoring of the water entering and exiting the Hovi wetland at 1-hour interval. The first full 1-year results (from November 2007 through October 2008) on the retention performance of the wetland were compared with the previous, water-sampling –based results [38].

## 3. Results and discussion

### *3.1. Performance of the network*

Several authors have discussed the reliability problems of WSNs. However, reliability is normally discussed from a technological perspective. Thus, diagnostic and debugging as well as communication protocols are analyzed in relation to the application and power-consumption [1, 21, 22]. These studies are important for recognizing missing measurements due to unreliable communication or sensor failure, but normally are unable to identify erroneous measurements. Sensor calibration and means to recognize and discard data from wrongly calibrated sensors has been also important aspect in ensuring data quality [8, 4].

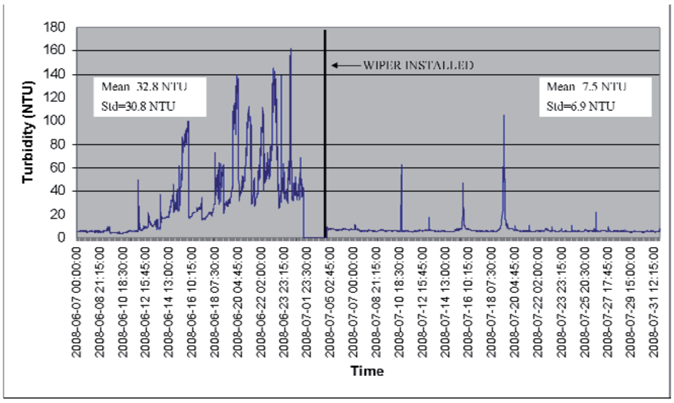
We analyze the performance of SoilWeather WSN by analyzing both missing and erroneous measurements, as well as the maintenance needed. The number and types of the maintenance visits are clarified and the problems with certain sensors are examined. The performance of the quality control is estimated by analyzing the number of erroneous and missing measurements. The better quality of the turbidity data is ensured by installing automatic cleaning wipers. The performance of turbidity wipers is analyzed by comparing turbidity values before and after the installation.

There are several factors related to the communication network, the stations or sensors themselves and the outdoor conditions that can interfere with the data. The improper functioning of the communication network can obstruct the data transfer and battery consumption. Under normal circumstances, the batteries should function properly for almost a year. However the strength of the signal within the GSM network can affect the battery age: a weak signal consumes more power from the station than a strong signal. Communication network problems can be seen as missing data or delayed data delivery.

Different problems can occur depending on the location of the station, weather conditions, nearby forest stand or the characteristics of the river. For example rain gauges tend to fill with leaves, tree needles and bird droppings thus distorting the precipitation data. In winter time the turbidity sensors might get broken due to moving ice. The first winter of the project was warmer than usually allowing the turbidity sensors to stay in the water for the whole winter without problems of freezing. In normal winter (as the second winter was) majority of the turbidity sensors has to be picked up for the coldest months.

Another problem concerning the turbidity measurements is the bio fouling of the optical lenses. Especially in summer time this is a big problem and the sensors would require cleaning on a regular basis, even daily in the most turbid waters. Also water plants, fish, gastropods or other objects in the water may affect the sensors. During the project we have discovered that almost without exception all the turbidity sensors need some kind of automatic cleaning system. At this point the wipers have been installed on the six sensors that have had most problems with biofouling or on sensors that are a long way from the MTT Vakola farm. The drastic effect of a wiper installed to a place that has normally very turbid water can be seen in Figure 7.

**Figure 7.** An example of the effect of a turbidity wiper installed to one of the SoilWeather WSN's turbidity sensors. Turbidity measures a month before and after the wiper has been installed. The mean and standard deviation before and after installation.




After the wiper has been installed, the level of turbidity has decreased dramatically. In addition there is no sign of the growing trend caused by the gradual contamination of the sensor. The real increase and level of the turbidity can now be seen in the data. The single spikes still remain in the data as they are caused by occasional disturbances. Obviously the mean value and standard deviation have decreased significantly in the study period. The cleaning of the turbidity sensors has probably been the most laborious maintenance task during the project. Furthermore the contamination of the turbidity sensors has caused most drastic errors to the data. With the help of the wipers these problems can partly be overcome.

In addition to maintenance of the turbidity sensors, battery problems have been quite major ones as well. Before the right composition of the battery package had been discovered, the gaps in the data were due to battery voltage decreasing or problems with battery contact. There have been five mysterious malfunctions of the stations as well. These stations had to be sent back to vendor and wholly repaired and reprogrammed. The main reasons for maintenance, how they occur in the data and how many occasions there has been during 1.5 years period are shown in Table 3.

**Table 3.** Maintenance intensity of SoilWeather WSN during 6/2007-12/2008.

| Problem | Manifestation in the data | Number of occasions |
|---|---|---|
| 1. Battery voltage decreasing | Missing data and/or air humidity decreases too much | 48 |
| 2. Turbidity sensor contaminated | Turbidity values too high and increasing | 64 |
| 3. Problems with battery contact | Missing data or station down | Ca. 40 |
| 4. Organisms on the turbidity sensor | Saw tooth pattern in the data | several |
| 5. Rain gauge clogged up | No accumulation of the precipitation despite of the nearby rain | 18 |
| 6. Station fell down | Possible problems with wind data and/or no precipitation | 12 |
| 7. Station malfunction | Missing data or station down regardless of battery condition | 5 |

The automatic quality control and warning system developed for detecting the most drastic errors has worked relatively well. Here we analyze the suspicious and erroneous measurements for period of four months, from July 2008 to October 2008. Only very small fraction (0.06 %) of the measurements was outside the range of the limit values. The total numbers of suspicious and erroneous measurements defined by the range test are shown in Table 4.

**Table 4.** Number of the suspicious and erroneous measurements by range test during 7/2008-10/2008.

| Parameter | Number of suspicious measurements | Number of erroneous measurements |
|---|---|---|
| Air temperature | 114 | - |
| Water level | 900 | 30 |
| Air pressure | 250 | - |
| Turbidity | 323 | 80 |

Air temperature was over the range limits for one station in one occasion due to few cold summer nights as the temperature decreased under the range value of 0 °C. Air pressure measurements have been below threshold value because of the decreasing battery voltage. In this case the problem was detected and solved fairly quickly. There have been 900 suspicious and 30 erroneous water level measurements. One of the water level sensors was for some reason pulled to the shore and another one was installed in a place whose water level decreased so much that it had to be moved to another spot. The total number of suspicious and erroneous turbidity measurements was ca. 400. These (mostly too high) turbidity measurements were caused by single spikes in the data.

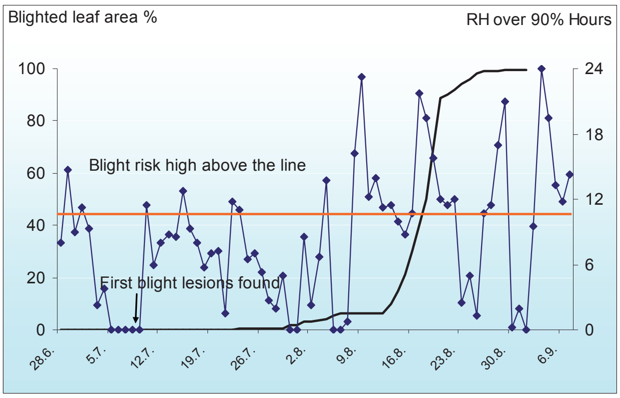
In general the sensor nodes and data transfer have been working well with regards to the missing values. At this point we only report the total number of problem occasions. Detailed analysis of lost data and their time span will follow later. For the weather stations the median of the proportion of the missing values was 0.6 % and for turbidity measurement stations 1.4 %. Due to different problems described earlier the variation was quite high: for some stations there have been missing values for over 10 % of the measurements. These missing values have usually been due to battery problems and therefore we have not found any differences according to the latitude component for example.

For good network functioning, it is essential that we are informed as soon as possible if some of the sensors or stations are not working at all. Altogether we still see the need to develop further the data checks and this way reach an optimal data flow and quality of the data. The present ability to detect the most obvious problems is a good start for this.

*3.2. Performance of applications*

Weather stations at the potato fields have been functioning relatively well. In the beginning of the season there were some technical errors in the measurement of relative humidity at some stations. The problems were solved and correct measurements were obtained during the critical period for potato late blight development. Blight risk at all potato fields was low until 9$^{th}$ of July. Between 10$^{th}$ and 25$^{th}$ of July there were 10 – 15 days when the temperature was over 8 °C and the relative humidity over 90 % for more than 10 hours. Blight risk was low from 26$^{th}$ July to 2$^{nd}$ August. From 3$^{rd}$ of August blight risk was very high until the end of August.

**Figure 8**. Duration of periods (hours), when relative humidity was more than 90 % and temperature over 8 °C and progress of potato late blight epidemic (percentage of defoliated leaf area) at Jokioinen in non-protected susceptible potato cultivar in 2008.




Blight was found at one field at the beginning of the high risk period 12$^{th}$ of July. After the high risk period the late blight was present in all fields at the end of July. During August the disease spread rapidly causing severe damage to three fields, where fungicide applications were started too late. In the rest of the fields blight was adequately controlled by fungicide applications. Blight risk estimated by duration of moist periods was relatively well in line with the observed blight epidemics.

In the field trial at Jokioinen blight progress was very similar to the potato fields at the SoilWeather network. Blight was found the 11$^{th}$ of July but the epidemic developed very slowly until August due to rather low blight risk. An epidemic exploded in the middle of August after several successive days when relative humidity was over 90 % more than 10 hours (Figure 8).

In wetland monitoring the turbidity sensors and the weather stations were used. In order to be accurate and reliable, automatic monitoring with sensors needs water samples for calibration of sensors for the specific conditions of the measurement place. Moreover, concentrations of some important substances –such as dissolved P– can not be measured with commonly available sensors thus leaving the laboratory analyses of the sampled water as the only option. In this study, a total of 75 samples were taken from the inflow water (24 manually and 51 with a refrigerator-equipped sampler). As for the outflow, 21 samples were taken manually during the 1-year study period. All water samples were analyzed for turbidity and the concentrations of TSS, total P (TP), dissolved reactive P (DRP) and nitrate (with nitrite).

The s::can sensors deployed in the Hovi wetland were calibrated using linear regression equations between the sample-based values and the simultaneous recordings of the sensors ("raw data"). Each recording of the raw data was then multiplied with the coefficient obtained by the regression equation of respective substance (turbidity or nitrate). Such calibrated values were used in the calculations of material fluxes. The final data curves were found to correspond well the sampled values [38], which suggested that the sensors functioned reliably.

Because turbidity does not represent an amount of substance in water it can not, like nitrate concentration, be directly used in the calculation of material fluxes. Fortunately, in the case of Hovi, correlations between turbidity and the concentrations of TSS and TP were very high with a coefficient of determination ($R^2$) of 0.86 or more. Thus, we could reliably transform the calibrated turbidity values into TSS and TP concentrations by multiplying them with the coefficients obtained from the linear regressions.

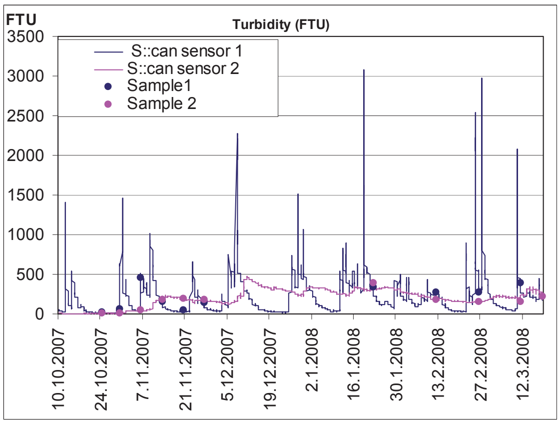
TSS and TP retentions in wetland (70 and 67%, respectively) were at a similar or slightly higher level than in the previous measurements. Meanwhile the value for nitrate retention (67%) was strongly increased. The improved nitrate retention suggests the positive effect of the vigorously expanded vegetation during the unmonitored time between the two study periods in the Hovi wetland.

Wetland measurements with sensors have been thus far successful. The information obtained with new technology has not only provided more accurate retention figures, but also given new insight on the behavior of TSS and nitrogen in a CW.

### *3.3. Benefits and challenges*

Due to the high temporal resolution of the measurements, SoilWeather WSN provides significantly more accurate information on nutrient leaching in different weather conditions at parcel level than can be achieved by regular sampling. Figure 9 shows turbidity measured with the spectrometer. The turbidity measured from water samples during the same time period indicates that most of the nitrate leaching peaks remains unnoticed highlighting the efficiency of sensor networks to monitor irregular, short events. The in-situ sensor networks provide point measurements that can be used as input in leaching models and, thus, improve the estimates of nutrient leaching at different scales.

**Figure 9.** Turbidity samples (dots) and turbidity measured by spectrometer (solid line) from the constructed wetland of Hovi.




The potato late blight forecast can be applied to justify precise timing of fungicide applications. In the future, forecasts for other crops and pests should be developed. Relatively good models that predict *Sclerotinia* diseases of oil seed crops exist [39]. More effort is needed to develop applications for cereal diseases while there is clear demand for such forecasts among farmers and advisors.

On the other hand, as the SoilWeather WSN provides over 30,000 measurements per day and data accumulates progressively over time, this poses significant data processing challenges. Due to the large amount of data erroneous or missing measurements need to be tracked and when possible, also corrected by automatic algorithms. Protocols for error diagnostics and debugging of WSNs have been developed that notify when measurements are missing due to communication, device or software faults [21, 40]. Determination on erroneous measurements, in turn, is sensor and environment specific, and base on statistical calculation and regular calibration samples.

Good sensor data quality is a critical factor for data users. Evolving standardising and increasing joint use of sensor data has been seen to lead to unforeseen data availability in the future [4]. It is also more and more critical for data user combining different data sources to be informed of the quality of data by providing quality estimates for measurements and documenting data quality and the control procedure. Joint use of sensor networks and webs requires development of open standard protocols and interfaces as well as open source software products to discover and analyse sensor data from different sources [7, 4]. The internet based data services enable easy access to data and metadata by users and applications in the case of single sensor network. At the moment SoilWeather data is collected in two different servers and respectively in two web services provided by sensor vendors used. In addition, the download of the data tables needs to be done station by station. In the next phase of SoilWeather WSN, it is important to develop web services so that they support easy data access and use. Also data flows from sensors and calibration samples need to be integrated and easily available.

If the large amount of data poses challenges to the user of sensor networks, the maintenance of the large sensor network is a challenge for the data provider. The monitoring over a large area and especially the continuous sensing of water requires maintenance resources. The amount of the field work and maintenance costs may be the same as in field logger based sensing. The sensors measuring water quality need regular cleaning in the field and calibration samples need to be taken. Depending on the locations of the sensor nodes, one field worker can maintain 5-10 sensors per day. Total maintenance costs of the whole SoilWeather network including also laboratory analyses of water and soil samples, data transfer costs, and costs of replacement parts and batteries are not available yet. Still they should not be underestimated, because it plays a key role in ensuring the quality of sensor data.

Major strength of the SoilWeather WSN is the tight collaboration between three governmental research institutes, Agrifood Research Finland, the Finnish Environment Institute and the Finnish Meteorological Institute. This way we have been able to establish a multipurpose network requiring a wide range of expertise and to develop a wide range of potential applications. The network is also established in collaboration with private enterprises including sensor vendors, data users and service developers. The low costs of the weather stations make it possible for individuals, such as farmers, and for small organizations to participate in the sensor networks in the future. Admittedly, data provided by the network would be interesting for other sectors such as tourism and traffic as well.

Considering the maintenance efforts, increased collaboration, open standard protocols and interfaces are seen as being important in the future development of SoilWeather WSN. By collaboration it is possible to create a cost-effective monitoring system that covers wide areas, provides data of good quality from different types of sensors and encourages joint use of data. Maintenance costs are decreased if the work is done close to the sensor location, whereas synergy is obtained if data quality procedures and algorithms are defined and developed, and employed together over the large group of data providers. When the number of data providers becomes larger, the control over data quality decreases. Therefore it is important to ensure that the data collection, processing and data quality is well documented and delivered to the users.

However, this collaboration requires open and widely used technology and standards that enable integration of different sensors and sensor data and flexible integration of new sensor nodes as well as tools for storing, archiving and delivering of data. The Sensor web enablement (SWE) of Open Geospatial Consortium (OGC) provides the needed standards and tools. It is also increasingly tested in a range of applications from earth observation through satellites to delivery of hydrological data [7]. If this technology shifts to operative use, it would also enable the discovery and exchange of data on a larger scale, through organizations, sectors and countries.

In addition to challenges in data processing and field maintenance we see data sensitivity and the attitudes of data providers as a third challenge. Especially if data is to be made freely available through web services. In the SoilWeather network, data on water quality is available only for the participants of WSN, while the weather data is already publicly available. This is because we want first to ensure the good quality of water measurement data by fully operational quality control procedures. However, aquatic measurements are also considered more sensitive data than meteorological data. In the case of SoilWeather WSN, farmers often do not want nutrient leaching rates available for anybody to follow if there is even a minor risk that high rates could cause changes to the management practices of the farm. One should, however, notice that the aims of the authorities and farmers are more or less congruent:

both of them benefit from low nutrient leaching to the rivers. Thus, it is also a question of attitudes that hinder collaborative monitoring of water quality. The water quality data is also sensitive from the perspectives of other potential private data providers than farmers. These could be enterprises providing drinking water for example. The public sector, in turn, is already opening their large environmental databases and supporting joint use of data. For example, the Finnish Environment Institute has recently opened a web service, Oiva, which provides most of the hydrological and water quality data collected by the environmental authorities in Finland (http://www.ymparisto.fi/oiva, in Finnish).

## 4. Conclusions

The SoilWeather network is still in the initial phase of the operation. Thus, not all the maintenance and sensor calibration procedures (particularly for soil) are fixed and data quality control algorithms for water and soil measurements are under the development. It is already clear that relatively high maintenance resources and effective data quality control are needed. However the maintenance efforts of the SoilWeather WSN can be decreased to some extent by the efficient organization of work, with good collaboration and by technical development of sensors and automatic cleaning systems. The amount of field work needed in aquatic data collection is higher than in meteorological and terrestrial data collection and the amount of fieldwork needed is expected to be no less than on the conventional, sampling based monitoring.

At the moment, the automatic quality control tests run on the SoilWeather WSN reveal the most drastic errors in the data, and warn of missing data. However, there is a need for more sensitive tests. Tests that compare the values of neighboring stations would be effective in detecting the faults in precipitation data for example. Consistency tests, on the other hand, would test if different parameter values of the same station are physically and climatologically consistent. For example the values of turbidity and precipitation or turbidity and water level depend on each other.

In the future development of SoilWeather WSN, we have to address three major challenges: 1) a large amount of data, 2) cost-effective maintenance of WSN and 3) the sensitivity of the data and the attitudes of data-owners towards data sharing. These challenges from user and data provider perspectives need to be considered when building operational environmental monitoring systems over a large area. However, we see the benefits of continuous environmental monitoring, and the increased accuracy of provided data, large enough to motivate overcoming the challenges. Furthermore, challenges may be partly overcome by good collaboration and development of tools for data quality control and data processing. To ensure the quality of data and decrease the heterogeneity of measurements, there is a need for handbook for WSN data providers on how to carry out automatic monitoring of environment, particularly related to the water measurements.

SoilWeather WSN is currently functioning and funded on a project basis. A great challenge will then be to find sustainable longer term funding. The obvious options are governmental funding or funding through beneficial business models that are developed on the WSN.

**Acknowledgements**

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# II

# A PRACTICAL APPROACH TO IMPROVE STATISTICAL PERFORMANCE OF WFD MONITORING NETWORKS

by

Niina Kotamäki, Marko Järvinen, Pirkko Kauppila, Samuli Korpinen, Anssi Lensu, Olli Malve, Sari Mitikka & Juhani Kettunen 2018

Manuscript

# III

# STATISTICAL DIMENSIONING OF NUTRIENT LOADING REDUCTION - LLR ASSESSMENT TOOL FOR LAKE MANAGERS

by

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# Statistical Dimensioning of Nutrient Loading Reduction: LLR Assessment Tool for Lake Managers

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**Abstract** Implementation of the EU Water Framework Directive (WFD) has set a great challenge on river basin management planning. Assessing the water quality of lakes and coastal waters as well as setting the accepted nutrient loading levels requires appropriate decision supporting tools and models. Uncertainty that is inevitably related to the assessment results and rises from several sources calls for more precise quantification and consideration. In this study, we present a modeling tool, called lake load response (LLR), which can be used for statistical dimensioning of the nutrient loading reduction. LLR calculates the reduction that is needed to achieve good ecological status in a lake in terms of total nutrients and chlorophyll *a* (chl-*a*) concentration. We show that by combining an empirical nutrient retention model with a hierarchical chl-*a* model, the national lake monitoring data can be used more efficiently for predictions to a single lake. To estimate the uncertainties, we separate the residual variability and the parameter uncertainty of the modeling results with the probabilistic Bayesian modeling framework. LLR has been developed to answer the urgent need for fast and simple assessment methods, especially when implementing WFD at such an extensive scale as in Finland. With a case study for an eutrophic Finnish lake, we demonstrate how the model can be utilized to set the target loadings and to see how the uncertainties are quantified and how they are accumulating within the modeling chain.

**Keywords** River basin management · Water Framework Directive · Lake water quality modeling · Bayesian inference · Hierarchical modeling · Uncertainty

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## Introduction

Eutrophication is a major threat to freshwater ecosystems (Carpenter et al. 1998). In many places, nutrient loading from the catchment area into the receiving waters has increased substantially above natural levels due to human action. Concern about deterioration of the ecological condition of surface waters due to elevated nutrient levels, and other pressures, gave rise to the EU Water Framework Directive (WFD, European Parliament and Council 2000). For WFD work, each water body is classified into one of the five different quality classes (high, good, moderate, poor, and bad). The requirement is to have at least good ecological condition in all surface waters by 2027 at the latest. European water bodies have already been surveyed and classified to identify those lakes that violate the current eutrophication-related water quality standards.

Lakes vary in their characteristics which affect their responses to elevated nutrient level (Malve and Qian 2006; Jackson et al. 2007; Carvalho et al. 2013). Also the concentrations of total phosphorus (CTP) and total nitrogen (CTN) that pose a risk for reduced water quality vary between lakes. This is why different lakes sharing some core characteristics are grouped together to represent different lake types. Each group is given specific class limits for $C_{TP}$ and $C_{TP}$ as well as chlorophyll *a* (chl-*a*) concentrations.

The limits are determined in relation to reference sites, so the further the measured classification values are from the limits of the 'high' class, the more the lake is presumed to be under anthropogenic pressure.

The most effective way to tackle the eutrophication problem and achieve permanent good condition in lakes would be reducing external nutrient loading. In many developed countries, point source loading from industry and municipalities is no longer the main concern, following implementation of stricter environmental legislation and strengthening of the requirements for purification of sewage effluent discharges. Hence, the focus of loading reduction has to be on diffuse loading from different land use actions, mainly from agriculture (Carpenter et al. 1998; Antikainen et al. 2008). Reducing diffuse phosphorus and nitrogen loading ($L_{\mathrm{TP}}$ and $L_{\mathrm{TN}}$) requires changes in land use practices and creating structures that prevent leaching of nutrients from the catchment into the recipient lake. These all have high costs because of the large land areas involved. For this reason, it is necessary to know the adequate, cost-effective level of management actions. Above all, it is essential to estimate the amount of $L_{\mathrm{TP}}$ and $L_{\mathrm{TN}}$ that a lake system can tolerate, and how much the loading needs to be reduced from its present level.

To link loading levels to receiving water body quality, the predictive power of mechanistic or empirical water quality models can be used (Borsuk et al. 2002; Chapra 2003). The modeling approach should be chosen considering the purpose of the modeling and the availability of the data (Pätynen 2014). The scale of the required loading reduction in terms of nutrient levels in a lake can be identified using simple empirical mass-balance and nutrient retention models. Cheng et al. (2010) examined seven different phosphorus retention and nutrient loading models based on Vollenweider's (1968, 1975, 1976) studies. External nutrient loading has also been linked to biological factors, such as chl-*a* and phytoplankton biomass (Jeppesen et al. 2005).

Usually, empirical models are driven from large cross-sectional datasets which derive from national lake monitoring programs. Yet fitting a global-scale model with common parameters to all lakes does not sufficiently take into account the intersystem variability (Cheng et al. 2010; Reckhow 1993). Phillips et al. (2008) overcame the heterogeneity problem of a large European dataset by splitting the data to more homogenous groups according to lake morphometry. They fitted separate linear regression models to describe chl-*a*-nutrient relationships in these groups. An even more efficient way would be to use a hierarchical, multilevel model in which the whole dataset is grouped into intermediate hierarchy levels inside the model. The different hierarchy levels can be based on different ecoregions (Lamon and Qian 2008), landscapes (Wagner et al. 2011), or lake types (Malve and Qian 2006), or on any such features that may cause variance at the lake level in the processes of interest. The hierarchy of the model enables using the data both from the study lake and from the lakes with similar features to make the predictions. In hierarchical model, lakes within the same type are assumed to have similar chl-*a* response to changing nutrient concentrations. Also a dataset of a lake type covers a wider range of observations than that of a single lake.

The representation of a complex system with simple empirical models clearly makes estimating the model error essential, although it should also be done in more complex modeling (see Doherty and Christensen 2011). In practice, it is not enough to model only the possible outcomes, but it is also important to know the margins within which to operate when aiming to make sufficient reduction in the external loading. The uncertainty that is related to the WFD assessment results in the lake management and decision-making process should be better accounted for and treated more coherently (Nõges et al. 2009; Rekolainen et al. 2003; Hering et al. 2010; Clarke 2012). The idea of uncertainty in the implementation of WFD is parallel to margin of safety (MOS) concept in the US EPA total maximum daily load procedure (TMDL committee 2001). In both cases, uncertainty is acknowledged both in the models selected as well as in the results of models. The reduction of the MOS can potentially lead to a significant reduction in implementation cost, and thus high priority should be on selecting and developing models with minimal forecast error.

The uncertainty in water quality modeling arises from several sources: not only from the model structure and parameter uncertainty but also from the measurement error (Rode et al. 2010). The measurement error (or unexplained residual error) stems usually either from spatial and temporal variability of the environment or from erroneous analytical methods (Gronewold and Borsuk 2010). The uncertainty can be handled and incorporated into a formal decision analysis context with the probabilistic Bayesian methods (Malve and Qian 2006; Malve 2007; Gronewold and Borsuk 2009; Ramin et al. 2011). Bayesian inference also offers a way to incorporate prior and new information into the system.

In Finland, there are nearly 200,000 lakes. About 87 % of the lakes' surface area have been classified, i.e., all lakes with surface area over 1 km$^2$ (Finnish Environment Institute 2013). Over 700 of these lakes do not meet the WFD criteria for good ecological water quality. The large amount of the lakes makes the management planning challenging. Therefore, for general and directional lake management, there is an urgent need for simple and fast screening level methods that operate at realistic time scales and with sensible costs. In this paper, we introduce a lake load response (LLR) internet tool which we have been developed for helping the river basin managers to implement the WFD. LLR links the effect of the $L_{TP}$ and $L_{TN}$ on the $C_{TP}$, $C_{TN}$ and chl-*a* in a lake. Due to its Bayesian modeling framework, LLR gives probabilistic assessments of water quality. As LLR is tailored especially for the Finnish WFD work, it acknowledges the national lake typology and classification criteria in its predictions. LLR calculates the effect of nutrient loading on nutrient levels in a lake with models based on Vollenweider's (1968) retention model equation. It further links the loading levels to chl-*a* concentration with a chl-*a* model that builds upon the hierarchical linear model introduced by Malve and Qian (2006). In this study, we fit the chl-*a* model to the updated Finnish monitoring data with revised lake typology. Combining simple water quality models in the Bayesian modeling framework brings a significant improvement to the present situation where the Vollenweider's equation or traditional regression models are applied as such in the WFD work. The Bayesian approach provides a very intuitive way of summarizing the uncertainties associated with the data analysis and is therefore useful for river basin management planning. We demonstrate the use of the LLR by applying it to the assessment of an eutrophic Finnish lake. LLR enables estimating the lake-specific nutrient loading reduction and the confidence of the WFD compliance.

## Materials and Methods

### The LLR Tool

The lake load response (LLR) is an open access internet tool that has originally been developed for the Finnish lake management (http://www.lakestate.vyh.fi). Although LLR is tailored for the Finnish lakes, the method has been also applied in the EU-funded research project WISER (Water bodies in Europe: Integrative Systems to assess Ecological status and Recovery, Hering et al. 2013, http://www.wiser.eu/). During the project, the effect of $C_{TP}$, $C_{TN}$ and water temperature on chl-*a* in 461 European lakes was examined.

Firstly in LLR, the effect of external nutrient loading on in-lake nutrient concentrations is estimated using empirical nutrient retention model (Vollenweider 1968) (Fig. 1). Secondly, the effect of in-lake nutrient concentration on chl-*a* is estimated using hierarchical chl-*a* model. The uncertainties are estimated using the Bayesian inference (Gelman et al. 2003) and the MCMC simulations (Laine 2008). The lake is represented as a continuously stirred tank reactor (CSTR). Therefore, it is assumed that the lake is completely mixed, there are no concentration gradients, and the nutrient concentration in the lake is equal to the concentration which is leaving the lake. CSTR assumption compromises well in Finnish lakes that are usually very shallow.

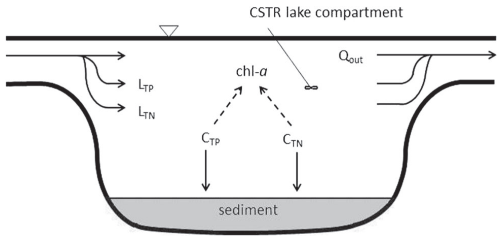


**Fig. 1** Conceptual diagram of the LLR variables including discharge, nutrient loadings, and in-lake concentrations

As input data, LLR requires information on $L_{TP}$ and $L_{TN}$ together with in-lake $C_{TP}$ and $C_{TN}$ and outflow ($Q_{out}$). If $C_{TP}$ and $C_{TN}$ observations are available from different parts of the lake, those from the main basin are used, and if samples are taken from different depths of the basin, the volume-weighted average is calculated. Further, because of the CSTR assumption, the loadings and the outflows are given as annual loading sums normalized to daily units. For lakes with long retention time, the loading is summed from a number of years equivalent to the retention time. In addition, information about lake's volume, mean depth, and lake type is needed.

As a result, LLR produces lake-specific statistical distributions of $C_{TP}$, $C_{TN}$, and chl-*a*; the target nutrient loadings; and the possible loading reductions. Results include the uncertainty estimates either as confidence regions or as a description of a distribution.

### Nutrient Retention Model

The nutrient retention model of LLR is based on the well-known Vollenweider steady-state mass-balance model (Vollenweider 1968, 1975, 1976) modified by Chapra (1975). The model requires lake-specific coefficients and it assumes that the in-lake nutrient concentration is equal to the external nutrient loading minus the outflow and the loss by sedimentation. Therefore, the in-lake $C_{TP}$, $C_{TN}$ (mg m$^{-3}$) can be expressed with $L_{TP}$, $L_{TN}$ (mg d$^{-1}$), $Q_{out}$ (m$^3$ d$^{-1}$), settling velocity ($v_s$, m d$^{-1}$), and the surface area of the lake ($A$, m$^2$).

$$C_{TP/TN} = \frac{L_{TP/TN}}{Q_{out} + v_s A} \quad (1)$$

The only unknown parameter in the model (Eq. 1) is the settling velocity ($v_s$) which can be determined with the other variables in the model. Instead of a single fit to the data, we can think that the settling velocity has a statistical distribution. This is a reasonable way of thinking as the settling velocity is usually poorly defined and the input data are noisy.

In other words, we will assume that the settling velocity and further the in-lake concentration, in the model (Eq. 1), vary randomly according to a normal distribution. The formulation of the model can now be summarized as follows:

$$C_{\mathrm{TP/TN}} \sim \mathcal{N}\left(f(v_s, x), \tau^2\right) \tag{2}$$

$$v_{\mathrm{s}} \sim \mathcal{N}\left(\mu_{\mathrm{s}}, \sigma_{\mathrm{s}}^2\right), \tag{3}$$

where the nutrient concentration from the lake ($C_{\mathrm{TP/TN}}$) is normally distributed ($\mathcal{N}$) with a mean value $f(v_{\mathrm{s}}, x)$ and an error variance $\tau^2$. The mean value is derived from the Vollenweider nutrient retention model ($f$) with the observed lake-specific input variables in vector $x$. The settling velocity $v_{\mathrm{s}}$ is normally distributed with a mean $\mu_{\mathrm{s}}$ and a variance $\sigma_{\mathrm{s}}^2$.

The parameter estimation is done according to the Bayesian framework where all the unknown parameters are first assigned a 'prior distribution' which describes the prior belief or knowledge about the unknown parameters (Gelman et al. 2003). The input data are then used to modify the prior distributions for each unknown parameter, to give 'posterior probability distributions'. For fitting the parameters to the data, we use inverse modeling package FME (Soetaert and Petzoldt 2010) in the R software package (R Core Team 2012). The uncertainty is assessed using a Markov Chain Monte Carlo (MCMC) algorithm with a delayed rejection and adaptive Metropolis procedure (Haario et al. 2006; Laine 2008). The retention model is first fitted to the input data, and the best-fit parameter estimate is used to initiate the MCMC chain. Therefore, we set the residual mean squares from the best fit as the initial model variance. Without better knowledge about the variation, we used the so-called non-informative prior distribution (i.e., all values are equally likely) for $v_{\mathrm{s}}$ estimation.

### Hierarchical Chlorophyll *a* Model

The estimated in-lake $C_{\mathrm{TP}}$ and $C_{\mathrm{TN}}$ (Eq. 2) can be used to predict the in-lake chl-*a* levels allowing the link between external loadings and chl-*a* to be estimated. In this study, we have fit the nutrient-chl-*a* model introduced by Malve and Qian (2006) to more recent monitoring data and updated Finnish lake typology. The typology is based on the principles specified in the EU WFD (CIS Guidance Document No 2 2005). According to the current Finnish lake typology (Pilke 2012; Juutinen et al. 2009), the naturally nutrient-rich (winter turbidity >5 FTU) and naturally calcareous (alkalinity >0.4) and Northern Lapland lakes are first distinguished. The rest of the lakes are then grouped into different types based on the surface area, mean depth, natural water color, and the retention time. The water quality criteria for good status have been defined for all lake types and for $C_{\mathrm{TP}}$, $C_{\mathrm{TN}}$ and chl-*a* separately (Table 1) following the ecological classification guidelines for Finnish lakes (Aroviita et al. 2012) which are based on WFD (CIS Guidance Document No 10 2003).

The data produced by the national Finnish water quality program are stored in a centralized database of the Finnish Environment Institute (Mannio et al. 2000). The sampling strategy and analysis methods have been described in Niemi et al. (2001). For the modeling, we collected a dataset that consists of 2246 Finnish lakes with a total of 36942 in-lake chl-*a*, $C_{\mathrm{TP}}$, and $C_{\mathrm{TN}}$ observations from July 1990 to August 2007. The surface area of the lakes ranges from 0.057 to 1377 km$^2$, mean depth from 0.29 to 20.8 m, and volume from 0.000086 to 14.9 km$^3$. The dataset includes several lakes of each lake type, from 9 calcium-rich lakes to 388 shallow humus-rich lakes (Table 1). There is obvious variation in the observed chl-*a*, $C_{\mathrm{TP}}$, and $C_{\mathrm{TN}}$ between and within the lake types (Fig. 2). The lowest chl-*a* median is in the northern Lapland lakes (1.7 μg l$^{-1}$) and the highest in nutrient-rich and calcium-rich lakes (type 12, median = 35.7 μg l$^{-1}$).

Malve and Qian (2006) showed that the chl-*a* variations in Finnish lakes can be predicted with $C_{\mathrm{TP}}$, $C_{\mathrm{TN}}$, and their interaction ($C_{\mathrm{TP}}$*$C_{\mathrm{TN}}$). Although $C_{\mathrm{TP}}$ is usually the most important determinant when assessing the amount of chl-*a*, $C_{\mathrm{TN}}$ can be more influential in non-humic lakes. We take these varying responses in nutrient-chl-*a* relationship into account using different nutrient intercepts and slopes for separate lake types. In practice, the chl-*a* predictions are almost solely based on data from the study lake when data are abundant, or if there is a very large scatter in the chl-*a* response to nutrient concentrations within lakes of the same type. If data from the study lake are insufficient, the predictions are based on the lake-type-specific data.

Our model (based Malve and Qian 2006) includes the overall mean for chl-*a*; the main effects of $C_{\mathrm{TP}}$, $C_{\mathrm{TN}}$, and their interaction; and the type-specific and lake-specific adjustments. The full form of the hierarchical linear chl-*a* model can now be summarized as follows:

$$\log(\text{chl - }a_{ijk}) = \underbrace{\beta_0 + \beta_1 \log(C_{\mathrm{TP}_{ijk}}) + \beta_2 \log(C_{\mathrm{TN}_{ijk}}) + \beta_3 \log(C_{\mathrm{TP}_{ijk}}) \log(C_{\mathrm{TN}_{ijk}})}_{\text{fixed effects}}$$
$$+ \underbrace{u_{0_{j/k}} + u_{1_{j/k}} \log(C_{\mathrm{TP}_{ijk}}) + u_{2_{j/k}} \log(C_{\mathrm{TN}_{ijk}})}_{\text{random effects of type}} + \underbrace{v_{0_{i/jk}} + v_{1_{i/jk}} \log(C_{\mathrm{TP}_{ijk}}) + v_{2_{i/jk}} \log(C_{\mathrm{TN}_{ijk}})}_{\text{random effects of lakes}} + \underbrace{\varepsilon_{ijk}}_{\text{error term}}, \tag{4}$$

**Table 1** Finnish lake types, concentration maxima of $C_{TP}$ and $C_{TN}$, and chl-*a* for good water quality and number of lakes (*n*) in chl-*a* model

| Number in LLR | Code | Name of the type | Criteria for good water quality | | | *n* |
|---|---|---|---|---|---|---|
| | | | $C_{TP}$ (μg $l^{-1}$) | $C_{TN}$ (μg $l^{-1}$) | Chl-*a* (μg $l^{-1}$) | |
| 1 | Vh | Small and medium low humic lakes | 18 | 500 | 7 | 375 |
| 2 | Ph | Small humic lakes | 28 | 700 | 15 | 343 |
| 3 | Kh | Medium humic lakes | 28 | 660 | 12 | 129 |
| 4 | SVh | Large low humic lakes | 18 | 500 | 7 | 67 |
| 5 | Sh | Large humic lakes | 25 | 600 | 11 | 46 |
| 6 | Rh | Highly humic lakes | 45 | 750 | 20 | 200 |
| 7 | MVh | Shallow low humic lakes | 25 | 600 | 8 | 82 |
| 8 | Mh | Shallow humic lakes | 40 | 750 | 20 | 384 |
| 9 | MRh | Shallow very humic lakes | 55 | 850 | 25 | 388 |
| 10 | Lv | Lakes with a very short retention time | 40 | 610 | 8 | 88 |
| 11 | PoLa | Lakes in northern Lapland | 12 | 300 | 5 | 11 |
| 12 | RrRk | Nutrient-rich and calcium-rich lakes (subtype not defined) | 55 | 930 | 20 | 57 |
| 13 | Rr | Nutrient-rich lakes (subtype of RrRk) | 55 | 930 | 20 | 68 |
| 14 | Rk | Calcium-rich lakes (subtype of RrRk) | 30 | 750 | 20 | 9 |

where chl-$a_{ijk}$ is chl-*a* concentration of sample *i* from lake *j* of lake type *k*. $\beta_0$, $\beta_1$, $\beta_2$, and $\beta_3$ are fixed global intercept and slopes of $C_{TP}$, $C_{TN}$, and their interaction. $C_{TP/TN_{ijk}}$ is the *i*th observation from lake *j* in lake-type *k*. $u_0$, $u_1$, and $u_2$ are lake-type-specific random intercepts and slopes for lake *j* of the type *k* (denoted as *j*/*k*). $v_0$, $v_1$, and $v_2$ are lake-specific random intercepts and slopes for lake *j* of the type *k* with observations *i* (denoted as *i*/*jk*). The residual error term for observation *i* from lake *j* in type *k* is $\varepsilon_{ijk}$.

We use terms 'fixed' and 'random' for model parameters such as they are used in a non-Bayesian statistical context of mixed effects modeling (e.g., Zuur et al. 2009). In the Bayesian analysis, there is no distinction between fixed and random effects as all unknown parameters are treated as random (Gelman et al. 2003). The only difference in the 'fixed' and 'random' effects is that their priors are determined differently. The beta parameters ('fixed') are assigned independent improper prior distributions and the *u* and *v* parameters ('random') have common mean and variance. The posterior distributions for all unknown parameters are generated with the observed summer time nutrient data using MCMCglmm package (Hadfield 2010) in the R software system (R Core Team 2012).

With the derived chl-*a* model parameter values and the estimated $C_{TP}$ and $C_{TN}$ from the nutrient retention model, chl-*a* with different loading values can be calculated. Because of the Bayesian modeling framework and MCMC simulations, the uncertainties that arise in LLR can be quantified. The uncertainties come from the parameter and residual error of the nutrient retention model ($\tau^2$ and $\sigma_s^2$ in Eqs. 2, 3) and from the residual error of the chl-*a* model ($\varepsilon_{ijk}$ in Eq. 4).

## Lake Kuortaneenjärvi

We demonstrate the LLR framework for Lake Kuortaneenjärvi in Western Finland (Fig. 3). The surface area of the lake is 14.6 $km^2$ and the mean depth is 3.7 m. The catchment area of the lake consists mostly of peat land and forest and the lake is highly humic (lake type Rh). The River Lapuanjoki runs through the Lake Kuortaneenjärvi which is influenced by the heavy nutrient loading from agriculture and forestry of the catchment. The lake acts as a natural sedimentation basin within the catchment, enhancing the water quality of the lower parts, whereas the lake itself has become eutrophic. The long-term (1991–2013) averages of $C_{TP}$, $C_{TN}$, and chl-*a* are 65, 893, and 28 μg $l^{-1}$, respectively, all exceeding the limits for good water quality of type Rh (Table 1). Based on the physico-chemical indicators and especially on the biological metrics (e.g., chl-*a*), the overall ecological condition of the lake is moderate.

As the lake is not in good ecological status, it is important to estimate the loading reductions and the probabilities of exceeding concentration criteria. As an input to LLR, we used the measured $C_{TP}$ and $C_{TN}$ from the deepest part of Lake Kuortaneenjärvi 1991–2013. As the external loadings to Lake Kuortaneenjärvi are not available from the measurements, we obtained them as well as the water outflow estimations of 1991–2013 from the operational watershed simulation and nutrient loading estimation model VEMALA (Huttunen et al. submitted) of the Finnish Environment Institute. VEMALA uses third-order catchment division as the spatial dimension and 1 day as the

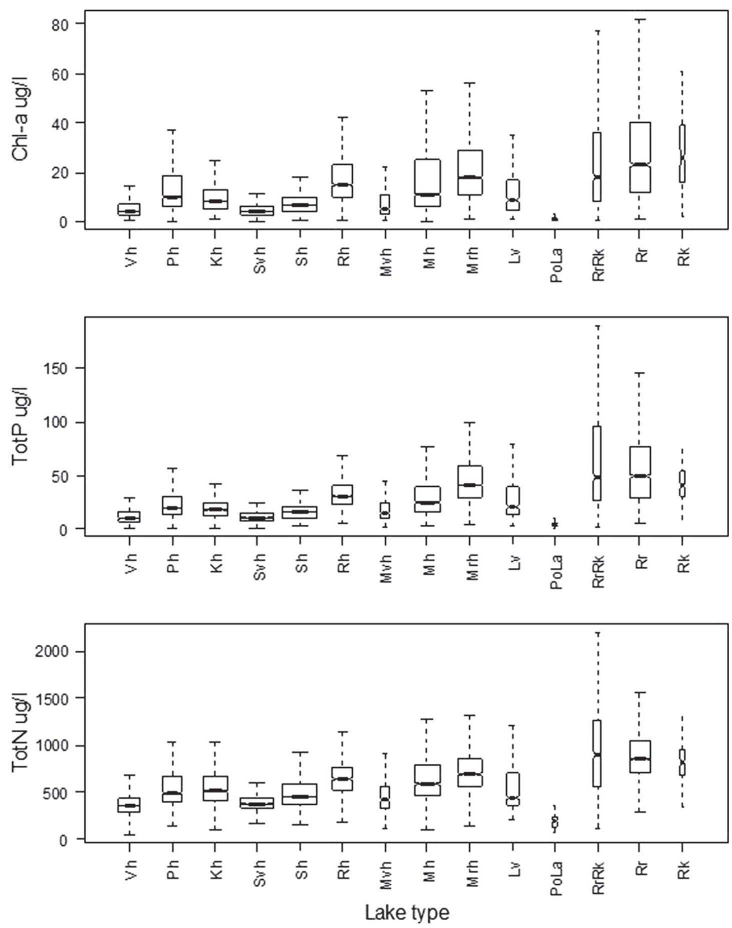


**Fig. 2** Observed Chl-*a*, $C_{TP}$, and $C_{TN}$ for different lake types in Finland. The *box plots* show the median, first, and third quartile ("hinges") and 95 % confidence interval of median ("notches"). The *box widths* are proportional to the square roots of the number of observations in the lake type

time increment and simulates the whole land area of Finland, including cross-border watersheds, and all the rivers and lakes (ca. 58,000) with an area of at least one hectare. VEMALA simulates the main components of the hydrological cycle, leaching of the total phosphorus, total nitrogen, and suspended solids from fields and forests and their transport in rivers and lakes up to the Baltic Sea. The nutrient loading sources are agriculture, forests, scattered settlements, and point sources. The diffuse loading simulation in the VEMALA version we have used is based on a regression model between nutrient concentration and runoff. The scattered settlements and point sources are included as input data. The nutrient loading calculation is calibrated by the nutrient observations. Therefore, the accuracy of loading estimates is highly dependent on the available observation time series. In case of Lake Kuortaneenjärvi, the frequency of needed measurements somewhat varied. Typically, (i) daily $Q_{in}$ observations, (ii) $C_{TP}$ and $C_{TN}$ measured four times a year from the incoming river discharge, and (iii) $C_{TP}$, $C_{TN}$, and chl-*a* measured four times in a summer from the lake were available.

## Results

### Chlorophyll *a* Model

The posterior distributions for all unknown parameters of the hierarchical chl-*a* model were obtained using MCMC simulations. A majority of the variation in the fixed effect is found in the intercept, followed by $C_{TP}$, $C_{TN}$, and the interaction (Fig. 4). Differences in the lake-type intercepts

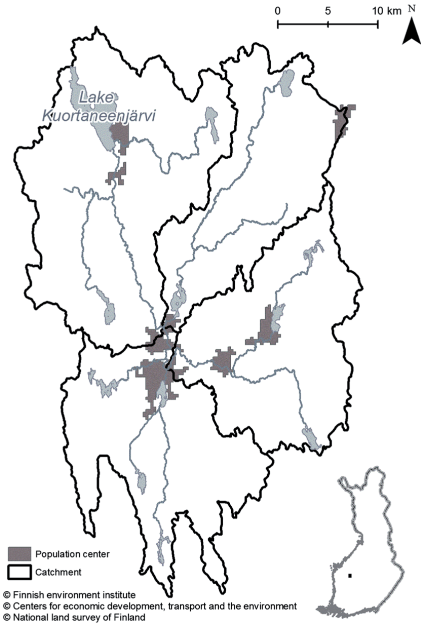


**Fig. 3** Map of Lake Kuortaneenjärvi catchment and Finland

illustrate different effects for different lake types. The intercept values of lake types correct the global chl-*a* value either upwards or downwards depending on their sign. For example, large humic lakes (Fig. 4b, type 5) show a larger lake-type intercept than other lake types. The lake-type slopes for $C_{TP}$ and $C_{TN}$ vary between lake types. The differences in the lake-type slopes effects are not as distinct as that for the intercept, although, e.g., for the northern Lapland lakes (Fig. 4c, type 11), the $C_{TP}$ effect is negative and varies more than in other lake types.

### Lake Kuortaneenjärvi Case Study

The nutrient retention model was fitted to Lake Kuortaneenjärvi's data and the relationship between the lake $C_{TP/TN}$ and $L_{TP/TN}$ was obtained (Fig. 5). The observed $C_{TP}$ is mostly around the Moderate/Poor class limit (65 μg $l^{-1}$). The observed $C_{TN}$ varies from good to poor level but most often it is in the moderate one. Because the parameter error and residual error of the nutrient retention models were calculated separately, we could differentiate their effects to the model prediction uncertainty. The uncertainty that rises from the model parameter error is substantially smaller than that from the residual error (Fig. 5).

Lake Kuortaneenjärvi's $C_{TP}$ and $C_{TN}$ probability distributions were obtained from the nutrient retention model with normally distributed settling velocity and model residual error (Fig. 6). According to the LLR results, the probability of achieving good status with the current average $L_{TP}$ level (1.45 g $m^2$ $a^{-1}$) is 4 %, thus the lake does not meet the WFD $C_{TP}$ criterion for good ecological water quality. The most probable phosphorus status is poor, with the probability of poor class being 51 %. According to $C_{TN}$, the most probable status with the long-term average $L_{TN}$ (2727 g $m^2$ $a^{-1}$) is moderate (45 %). The probability of achieving good status with the current loading level is 46 %.

For estimating the nutrient loading reduction, the relationship between external loading and in-lake nutrient concentration was derived with median outflow and external loading values varying from very small loadings to large (but possible) values (Fig. 7). In order to achieve good phosphorus status on average, the external $L_{TP}$ should not exceed 1.0 g $m^2$ $a^{-1}$ (Fig. 7a). Therefore, it should be reduced by 30 %. In case of $C_{TN}$, as the critical $L_{TN}$ is 23 g $m^2$ $a^{-1}$ (Fig. 7b), the required loading reduction should be about 13 %. From these results, we could make estimates on any confidence level. For example, if the required confidence of achieving the target is 90 %, or in other words, if the limit is exceeded with a probability of 10 %, then the $L_{TN}$ reduction should be about 60 %.

Possible effects of nutrient loadings to chl-*a* level can be examined by the lake-specific contour lines simulated with the chl-*a* model (Fig. 8a). The nutrient loadings were extrapolated for a larger range than that of observed in the Lake Kuortaneenjärvi. This is statistically justified in the case of a hierarchical regression model, where the lake-type observations cover a larger range than in a single lake. With low $L_{TP}$ and high $L_{TN}$, the contour lines are parallel to y-axis indicating phosphorus limitation within this range (Fig. 8a). On the other hand, with high $L_{TP}$ and low $L_{TN}$, the $L_{TN}$ reductions would affect the chl-*a* level most. With given average of annual daily loadings (asterisk in Fig. 8a), the median chl-*a* is 25 μg $l^{-1}$ exceeding the good chl-*a* criteria for this lake type (20 μg $l^{-1}$). Both $L_{TP}$ and $L_{TN}$ reductions affect the chl-*a* level helping to achieve the good level.

Substituting the estimated lake-type and lake-specific parameter values and the median values of simulated nutrient concentration distributions to the chl-*a* model the chl-*a* distribution with given loading values was calculated. This predictive probability distribution of chl-*a* (Fig. 8b) shows that the lake is in moderate condition (100 %).

At a moment, our chl-*a* model accounts only for the residual variance in the chl-*a* model. Considering also the nutrient retention model residual variance, the predictive posterior variance of chl-*a* increases considerably. For illustrating this effect, we substituted the 25th and 75th percentiles (in addition to median values) from the

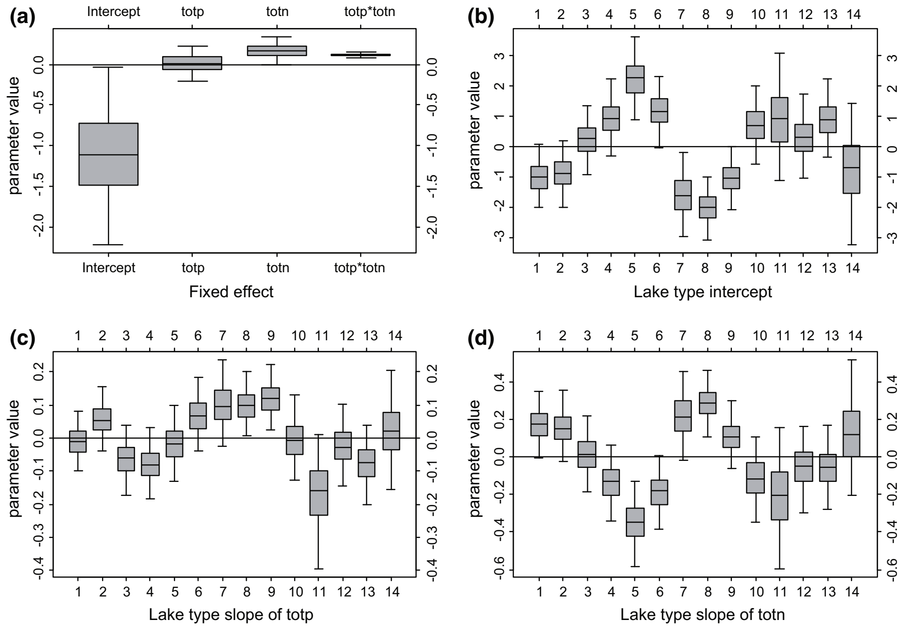


**Fig. 4** Chl-*a* model posterior *box plots* for **a** the unknown fixed effects and **b** lake-type intercepts, **c** lake-type slopes for $C_{TP}$, and **d** lake-type slopes for $C_{TN}$

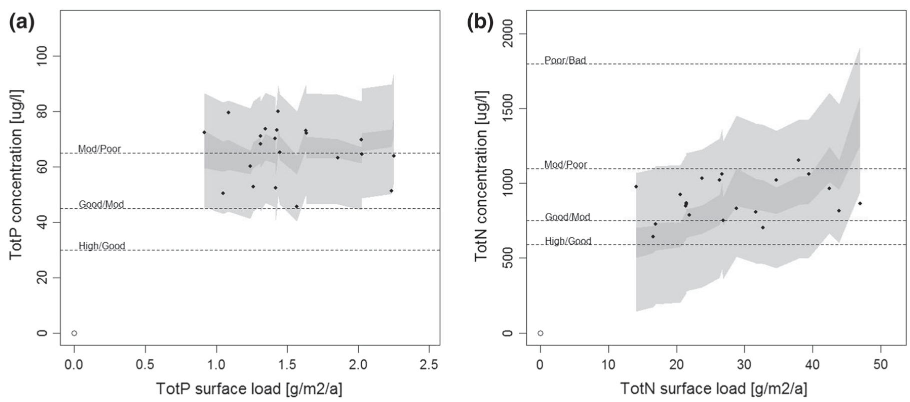


**Fig. 5** Model fit of the retention model for **a** $L_{TP}$ and **b** $L_{TN}$. The 90 % model parameter uncertainty as *dark gray*; the 90 % parameter uncertainty and residual error together as *light gray*. The observed values are shown as *dots* and *horizontal dashed lines* denote the status class limits

simulated $C_{TP}$ and $C_{TN}$ distributions to the chl-*a* model. The predictive chl-*a* distribution is now larger and the probability of the lake being in moderate condition is 73 % and the probability of achieving the target chl-*a* (20 µg $l^{-1}$) is 25 % (Fig. 9).

## Discussion and Conclusions

The link from external nutrient loadings to the lake's ecological status (determined here by chl-*a*) is a key to solve the problem of estimating loading responses and needed loading

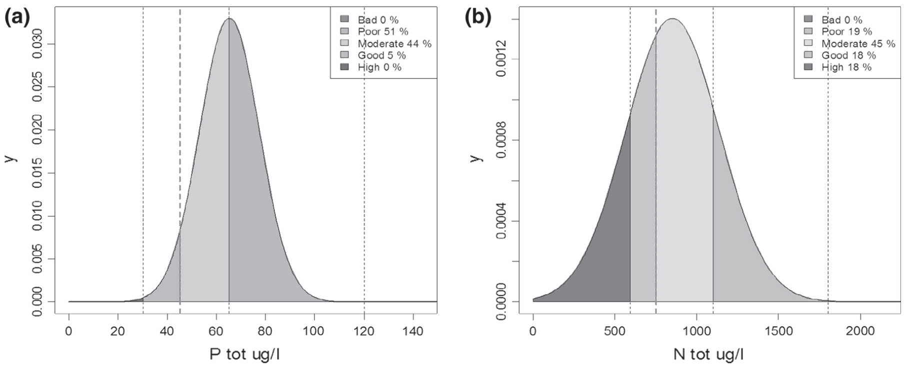


**Fig. 6** Predictive probability distributions of **a** $C_{TP}$ and **b** $C_{TN}$ with current $L_{TP}$ and $L_{TN}$. Different *colors* denote different WFD status classes and the proportion of the *color* denotes the probability with which the status is achieved

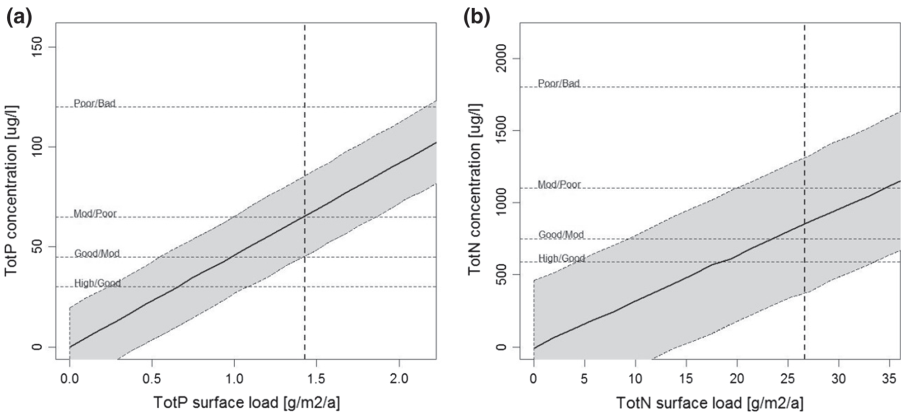


**Fig. 7** In-lake **a** $C_{TP}$ and **b** $C_{TN}$ as a function of $L_{TP}$ and $L_{TN}$ with median estimates and 90 % confidence regions. Observed median loadings are shown as *broken vertical lines* and status class limits as *horizontal lines*

reductions. With LLR, we could quantify these effects by combining the well-known Vollenweider nutrient retention model to hierarchical chl-*a* model. Using a hierarchical model, structure allowed us to include into our model all the available information, of which some might apply regardless of the lake type. This enhances the possibility for predictions outside the range of observations from a single lake.

The posterior box plots in our study show that for some groups the intercepts and slopes are similar, but for some other groups they can vary a lot suggesting that some groups could be combined to gain more group-specific data. On the other hand, the lakes in northern Lapland are too heterogeneous for discrete generalizations. Although LLR is tailored for WFD lake types, it has to be admitted that the Finnish lake typology is not optimal for hierarchical modeling as pointed by Lamon (Lamon et al. 2008). We need to consider this in the LLR development and instead of using the lake types in the hierarchy we should utilize the metrics used to create the typology.

The nutrient retention model results for Lake Kuortaneenjärvi showed that nearly all the modeled values are inside the 90 % confidence intervals. Therefore, both nutrient models fit the lake-specific data rather well. However, the observed values are from quite a narrow range, which makes the predictions uncertain outside the observed range. As for most lakes in Finland, there are no measurements of the external loading for Lake Kuortaneenjärvi and the ranges of the observed values are too narrow for reliable predictions. This is a recognized shortcoming of the nutrient retention model in LLR. We can obtain simulated loading values from hydrological loading models (such as VEMALA) as LLR input, but those do not fully

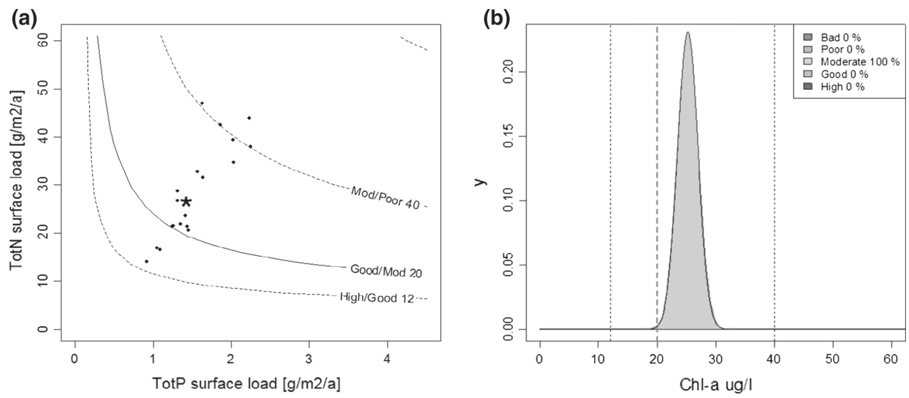


**Fig. 8** **a** Contours of chl-*a* showing the median chl-*a* estimate with different $L_{TP}$ and $L_{TN}$ combinations for Lake Kuortaneenjärvi. *Asterisk* indicates the median chl-*a* estimate with median loadings and *dots* the observed loadings. **b** Predictive probability distribution of chl-*a* with median $L_{TP}$ and $L_{TN}$

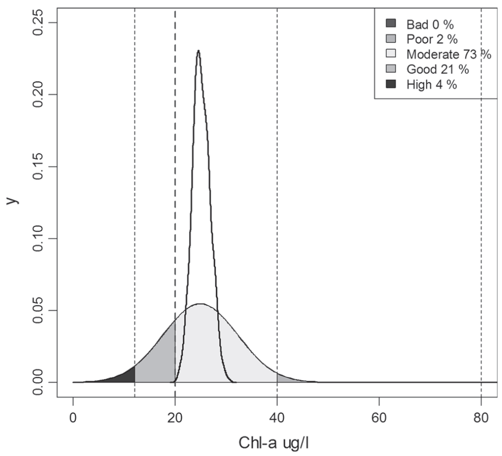


**Fig. 9** Predictive probability distributions of chl-*a* concentration when only the hierarchical chl-*a* model prediction uncertainty is accounted (*narrow bold line*) and when the nutrient model parameter and residual uncertainty are accounted for. For the latter, different *colors* denote different WFD status classes and the proportion of the *color* denotes the probability with which the status is achieved

compensate for true measurements. Most importantly, with more comprehensive nutrient balance data, we could improve the nutrient retention model performance. Fitting the retention model in the hierarchical Bayesian framework would help transfer information across different lake types and therefore support the predictions in lakes with narrow range of observations (Cheng et al. 2010). For this purpose, we have already started to collect nutrient balance data from Finnish lakes. Unfortunately, these data are scarce, due to the high costs and laboriousness of their collection at the moment. In addition, the highest loading events often happen outside the growing season, and are related to high runoff events and un-vegetated ground (especially fields). There can be high inter-annual variation in the timing and amount of loading due to differences in rain events and temperatures during autumn-spring, which makes loading assessment challenging (Puustinen et al. 2007). Currently, we have a dataset of nutrient balances from 12 lakes sufficiently well documented to be used as a basis for loading-lake response predictions. Since it is known that nutrients are the main cause of eutrophication, even more effort needs to be put into studying the external nutrient loading and its sources. Hopefully, as the importance of the issue is acknowledged and automatic monitoring techniques are developed, more data will become available for building up more reliable loading calculations.

However, with many eutrophic lakes, the external loading is not the only source of nutrients, and thus does not completely explain the in-lake nutrient concentrations. Obviously, this hinders predictions of the target loading. For instance, it has been estimated that the amount of phosphorus released from the sediment of Lake Kuortaneenjärvi during summer is approximately half the amount of the external loading. The effect of this internal loading can also be seen in the phosphorus model fit where an increase in the external loading does not significantly affect simulated $C_{TP}$. Taking into account the internal loading is already in progress in the LLR development.

The validity of the loading values is also significant for reducing the uncertainty that arises from several sources. Although using a hierarchical model structure in the chl-*a* model increases the model accuracy compared to the traditional regression models (Malve and Qian 2006), the variation in the input data and the parameter and residual errors in the nutrient models bring a significant amount of uncertainty to the chl-*a* distribution. Therefore, we should acknowledge that the median value from the nutrient retention model used for chl-*a* predictions also has uncertainty. Calculating the chl-*a* distribution not only with the median nutrients but also with the variability attached to them gives a better estimate of the unexplained residual uncertainty, which in the case of Lake Kuortaneenjärvi is considerable. We need to improve the loading monitoring in order to reduce the uncertainty and to improve the efficiency of management.

Despite the many aspects that need to be improved in the LLR tool, there is an urgent need for such fast and simple assessment tool for use in implementing the WFD, especially at such an extensive scale as in Finland. Although we are planning to develop LLR further, the aim is to keep it relatively simple to use and the data requirements modest. Currently, target nutrient loadings have been calculated with LLR for at least 50 lakes in Finland. Our study shows that the simplified modeling approach together with Bayesian inference offers a powerful tool for the decision-making process in the river basin management.

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# IV

# CAUSAL ANALYSIS OF PHYTOPLANKTON DEVELOPMENT IN A SMALL HUMIC LAKE USING STRUCTURAL EQUATION MODELLING

by

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Article

# Causal analysis of phytoplankton development in a small humic lake using structural equation modelling

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## Abstract

The factors affecting phytoplankton development in a small boreal, dystrophic lake during summer stratification were explored using structural equation models (SEM). Phosphorus had the highest positive impact on phytoplankton, and higher temperatures also enhanced the biomass. Water colour, and to a lesser extent intense zooplankton grazing, restricted phytoplankton biomass. Grazers generally seemed to be ineffective at controlling phytoplankton, however, which could be partly due to the high abundance of *Gonyostomum semen* (Raphidophyceae), a large motile algae not readily grazed by zooplankton. The importance of water colour, a significant factor in dystrophic lakes, emerged clearer in SEM than from regression models. SEM proved to be an effective and informative technique for exploring the factors affecting phytoplankton development, the role of each variable, and their interactions. Incorporating Bayesian analysis into the traditional SEM enabled a more detailed examination of variation in the variable estimates and possible sources of uncertainty and provided more reliable error estimates. We used total chlorophyll *a* as a proxy for total phytoplankton biomass, but the results clearly indicated that some of the emerging questions could have been better addressed by separating different phytoplankton groups. Nevertheless, SEM provided new insights from standard data, and we encourage its further applications in aquatic science.

**Key words:** boreal lakes, chlorophyll *a*, path analysis, water colour

## Introduction

Many lakes in the boreal region are dystrophic with high concentrations of coloured dissolved organic matter (CDOM) and iron. The resulting brown water colour affects light penetration into the lake. In addition, the surface of brown water lakes absorbs heat more efficiently, which may lead to stronger stratification and alterations to the thermal structure (Mazumder and Taylor 1994, Houser 2006, Arvola et al. 2010). There has been a rising trend in the concentration of dissolved organic carbon (DOC) together with water colour in the lakes of Nordic regions recovering from acidification (Monteith et al. 2007). In addition, the warming climate is predicted to further increase the leaching of DOC and humic substances from peat land and forested catchments into the lakes (Freeman et al. 2001, Naden et al. 2010). This on-going brownification of lakes is highly relevant to phytoplankton because it will decrease the depth of the euphotic zone and may constrain primary production (Carpenter et al. 1998, Arvola et al. 2014).

Likely changes in stratification may also be significant. Phytoplankton communities in small dystrophic lakes are often dominated by flagellate taxa (e.g., Arvola 1986, Lepistö and Rosenström 1998) that can regulate their vertical position in the water column (Salonen et al. 1984, Smolander and Arvola 1988) and which may also be able to avoid grazers to some extent. All these issues affect the

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intervariable relationships within the ecosystem and complicate the analysis of variable interactions.

Lake Valkea-Kotinen in southern Finland is a national long-term ecological research (LTER) site where the concentration of DOC and water colour have increased from 1990 to 2009 (Vuorenmaa et al. 2014). Although negative correlations between water colour and phytoplankton (biomass, primary production, and chlorophyll *a*) were detected, in stepwise regression analysis the possible effect of colour was unclear (Peltomaa et al. 2013, Arvola et al. 2014). Moreover, the influence of zooplankton grazing on the phytoplankton in Lake Valkea-Kotinen is not known in detail (Arvola 2014 and its references) and should be further examined, although we would expect grazing, like colour, to decrease the phytoplankton biomass (Carpenter et al. 1998).

The use of linear regression to explain the interactions between variables is common in ecology. Due to uncontrollable variation, heterogeneity, auto-correlation, and gaps or zeros in environmental monitoring data, however, linear regression may not be the best option among other routinely applied statistical methods (Whittingham et al. 2006, Zuur et al. 2010). The assumptions of linear regression, which in practice the data seldom meet, are ignored at the expense of analytical power. To obtain maximum benefit from long-term monitoring data and reveal the variable interactions and underlying patterns (Bolker et al. 2009), some more appropriate methods could be applied. Hence, we took a different approach to study the factors affecting phytoplankton development in Lake Valkea-Kotinen by using structural equation modelling (SEM). SEM is widely used in psychology and economics and is increasingly used in ecology (Pätynen et al. 2013). The method has also shown potential for use in phytoplankton studies (Arhonditsis et al. 2006, 2007a, 2007b, Liu et al. 2010, Salmaso 2011). SEM is able to process difficult data that are autocorrelated, non-normal, or even incomplete. Problems with sampling error (statistical) and variation can also be overcome. Even more appealing is the basic property of SEM that enables examination of not only the causal relationships between several variables, but also the importance of each variable separately (Shipley 2002). Thus, examining its applicability and evaluating its suitability for wider use within aquatic studies would be valuable.

We tested the applicability of SEM for deeper (and more statistically correct) examination of variable interactions in Lake Valkea-Kotinen than that gained through linear regression. We particularly explored whether SEM would identify colour and grazing as important negative factors for phytoplankton development in Lake Valkea-Kotinen. In general, we aimed to gain deeper insight into the interactions between phytoplankton of a small dystrophic lake and the variables that have been routinely measured: water colour, nutrients, temperature, and zooplankton. To our knowledge, until now SEM has not been applied to this kind of environment; hence, our study provides additional information regarding its performance and utility. By incorporating Bayesian analysis into SEM and by examining the posterior distributions, we expected to gain additional information about the different variables and the uncertainties associated with them as well as improve the modelling by allowing smaller sample sizes (Arhonditsis et al. 2006) and providing more reliable error estimates.

## Materials and methods

### Study area and data

Lake Valkea-Kotinen is a small headwater lake (area 0.042 km$^2$, mean depth 2.5 m, maximum depth 6.5 m) in southern Finland (61°14′32.1″N; 25°3′46.5″E). The lake is surrounded by a forested catchment and can be considered a reference site due to low anthropogenic influence, which is especially beneficial in modelling studies because of fewer interfering factors. The organic carbon load from the catchment gives the lake a noticeably brown colour (1990–1995 median of 134 mg Pt L$^{-1}$). Because of its small size and sheltered position, the lake is dimictic and produces a steep thermal and oxygen stratification in the summer, with a 1.5–2 m thick epilimnion. The depth of the euphotic zone is approximately the same (Peltomaa and Ojala 2010), so we focused our study on the water layer at 0–2 m. Because of the strong seasonality and distinct differences between summer and winter conditions (the sampling frequency decreased during winter), we included only measurements from the ice-free period. Further, we considered only the period between the overturns in spring and autumn; thus, from each year the first and last sampling dates were included when the temperature difference between the surface and the bottom layer was >2 °C.

For the modelling, we utilized data collected as a part of the long-term monitoring of Lake Valkea-Kotinen. The epilimnetic samples for concentrations of chlorophyll *a*, nutrients (total phosphorus, total nitrogen, $PO_4$-P, $NO_3$-N, and $NH_4$-N), water temperature, and colour were from 0 to 1 m and 1 to 2 m in 1990–1995. Data from some sampling occasions had to be omitted because 2 of the methods applied for parameter estimations (generalized least squares and asymptotically distribution-free estimates, discussed later) do not permit missing values. We also had counts for 3 zooplankton groups: cladocerans, copepods, and rotifers. The zooplankton sampling differed in that 2 parallel samples were taken at 1 m intervals from the surface to 5 m depth and pooled for a combined sample.

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Because the zooplankton data were strongly skewed, we transformed it using natural logarithms. More detailed descriptions of the sampling and analyses can be found from Peltomaa et al. (2013), Arvola et al. (2014), and Lehtovaara et al. (2014).

### Structural equation modelling

We used the AMOS software of SPSS for SEM to study the effects of different variables on phytoplankton development in Lake Valkea-Kotinen. Because the technique has received limited attention within aquatic sciences, we briefly describe the different SEM steps used in our study. We first created a conceptual model of the variables to be included in the SEM based on previous knowledge of the processes taking place in lakes in general. Hence, our model was confirmatory because our aim was to validate a hypothesis about the system function using SEM. In a more dynamic modelling process, SEM could also be used as an exploratory tool to develop new hypotheses and test them through experiments or further observation and, finally, with a confirmatory model.

SEM has 2 types of variables: observed and latent. The benefit of latent variables is that they can be unmeasurable, yet (preferably) describable through measured variables (Shipley 2002). The inclusion of latent variables also captures the unreliability of measurements in the model and distinguishes SEM from simple paths analysis (which can be considered a special case of SEM). For example, in our model we used chlorophyll *a* to model the latent variable "Phytoplankton" because it is known to serve as a proxy for phytoplankton abundance, yet does not completely describe it. To gain tentative information about the variable interactions and how they could be grouped to form latent variables, we examined the Lake Valkea-Kotinen data with principal component analysis and linear regression. SEM was finally created with the selected variables, creating paths between different variables and the direction of effects as well as indicating probable correlations between them (Fig. 1).

After establishing the SEM, estimates for the paths (parameters) were calculated with the help of maximum likelihood estimation (ML), generalized least squares (GLS), and the asymptotically distribution-free (ADF) method, so that the model was able to create a variance–covariance (or correlation) matrix for the variables, congruent to the one observed (Hershberger et al. 2003). The null hypothesis ($H_0$) in SEM is that the observed covariance matrix equals the model-implied matrix, and the model can be accepted; hence, an important feature for interpretation of results is the acceptance, not rejection, of $H_0$.

One assumption of the ML estimation, which is most often used for parameter estimation in SEM, is multivariate normal data, yet non-normality of observational data is unfortunately common. The zooplankton data were ln-transformed because they were strongly skewed for all zooplankton groups, but transforming total phosphorus and especially the chlorophyll *a* data would also have been necessary to gain multivariate normality for the whole dataset. Transformation of chlorophyll *a* was not possible, however, because it led to identification problems in the model (i.e., with parameter estimation). Because non-normality increases the risk of type 1 error (rejecting a valid model), we used ML for estimates but also used GLS and ADF for comparison.

We performed a $\chi^2$ test in AMOS to confirm the congruity between the observed and modelled matrices. Accepting $H_0$ means that the $\chi^2$ test value should be as small as possible, degrees of freedom should be high, and $p > 0.05$ (e.g., Shipley 2002, Hershberger et al. 2003, Grace et al. 2010). Eventually we tested several possible models with slight variations in the included variables, repeating the process from the development of the SEM to the $\chi^2$ test, before the best model was selected for this research.

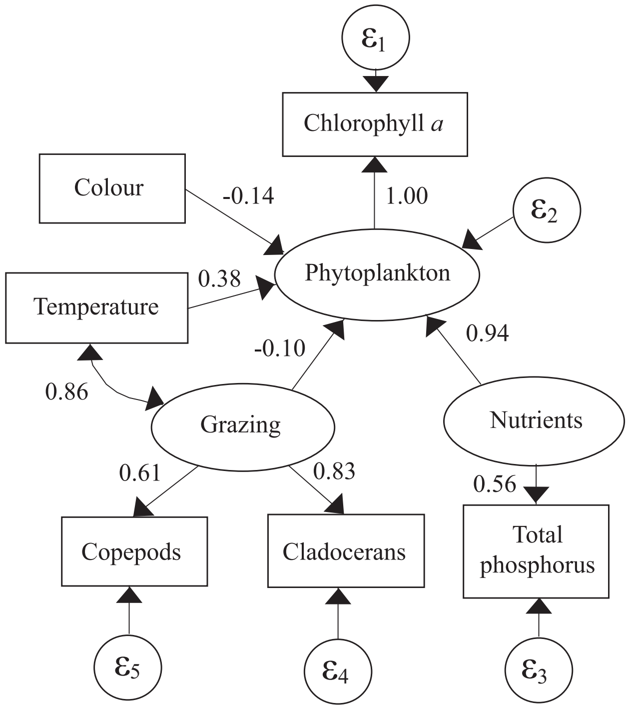


**Fig 1.** Structural equation model for Lake Valkea-Kotinen (n = 144). Measured variables are indicated with rectangles, latent (unmeasured) variables with ovals, and error terms with circles. Arrows indicate the direction of effects, and 2-headed arrows indicate correlation between variables. Numbers beside each arrow indicate the standardized path coefficient, or regression weights between variables, estimated using maximum likelihood. A $\chi^2$ test of the congruence between the measured and modelled correlation matrices yielded a $\chi^2$ value of 15.741 (10 df, $p = 0.107$).

After constructing a model with the help of the other techniques, we performed Bayesian analysis to obtain more realistic estimates for error term variances for zooplankters and total phosphorus, and thus to improve the Lake Valkea-Kotinen SEM, by leaving the variances unconstrained (not setting them as 1). After obtaining the variance estimates, we set them as constraints in the conceptual model and performed new estimates with ML, GLS, and ADF, which are presented as final results. Bayesian SEM does not rely on asymptotic theory, which allows smaller sample sizes (Arhonditsis et al. 2006) compared with traditional SEM in which the number of observations should be 200 or more (Shipley 2002), a value not reached with our data ($n = 144$). Also, confirmation of the results with ML, GLS, and ADF was appropriate. The variances in posterior distributions of Bayesian analysis yielded additional information about the different variables and uncertainties associated with them, which can then be used to decide which variables should be measured more frequently for better model accuracy and to better answer questions of interest. Bayesian analysis can also indicate multimodality in the estimations, which may be relevant for interpreting results. In this study we did not add prior information into the Bayesian analysis, but instead used flat, uninformative priors and let the data drive the process.

Because the datasets in some earlier studies (e.g., Arvola et al. 2014) were not identical to ours, we also created a regression model for better comparison between SEM and linear regression. The data and the included variables were exactly the same as in SEM.

## Results

The final SEM for Lake Valkea-Kotinen included nutrients (total phosphorus) and grazing (cladocerans and copepods) as latent variables, and temperature and water colour as measured variables that together had the strongest effect on phytoplankton (Fig. 1). The correlation between temperature and grazing was strong and was thus included in the model. All other variables, including the other nutrient fractions and the rotifers, were excluded from the final model because they were not supported by the data. The correlation matrices (Table 1) and estimates with different methods (ML, GLM, and ADF) supported each other (Table 2), and the $\chi^2$-test values indicated equally good model fits for each of them (Table 3). The Bayesian analysis supported the other estimates and indicated that the highest uncertainty derives from the biological variables because their deviation in posterior distributions increased (Table 2). Using the error variances estimated with the Bayesian method for ML, GLM, and ADF estimates slightly improved the $\chi^2$-test values for the final SEM (Table 3).

In SEM, the direct paths between different variables can be examined for direction and strength of their interactions. The standardized path coefficients between variables are equivalent to the standardized regression weights (Fig. 1), and, similarly, regression $p$-values can be calculated for each path to better evaluate the importance of each variable independently (Table 2). When latent variables are included, however, the total standardized effect of measured variables on the dependent variable is calculated by multiplying the effect between the measured and latent variable by that between the latent and dependent variable. Hence, a positive effect of total phosphorus and temperature on phytoplankton development in Lake Valkea-Kotinen was found (Fig. 1; Table 2). In contrast, the negative effect of colour and zooplankton (grazing) is not as strong; colour seems to be a more influential factor, while the total standardized effect of cladocerans on phytoplankton can be calculated as $0.83 \times (-0.10) = (-0.08)$ (Fig. 1; Table 2).

In the regression model, the effect of total phosphorus and water temperature on chlorophyll *a* was significant (Table 4). The effect of colour was negative, with an acceptable significance level ($p = 0.044$). There was no clear effect of either cladocerans or copepods on chlorophyll *a*, and the adjusted $R^2$ for the overall model was 0.40.

## Discussion

We created SEM that revealed the selected variable interactions in Lake Valkea-Kotinen. According to our SEM analysis, water temperature and nutrients explained most of the phytoplankton biomass development in the lake. The positive effect of water temperature and nutrients was higher than the negative effects of colour and grazing; the effect of grazing was especially more distinct with SEM than in a regression model. The possibility to add correlations (and interactions) between explanatory variables improved the description of the studied system. The biggest differences between our SEM and the stepwise regression presented by Arvola et al. (2014) was that the latter excluded temperature altogether, and the effect of zooplankton was not taken into account. The inclusion of zooplankton in our regression model is also poorly justified (see individual p-values in Table 4) because it did not further improve the model. If a stepwise method had been used instead of entering the selected variables, cladocerans and copepods would have been omitted from the model.

The questions and the conceptual model could involve only the measured variables (or those latent variables that could be described with the measured variables), which kept our SEM simple and limited the study questions. We

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**Table 1.** Correlation matrix for variables in the Lake Valkea-Kotinen structural equation model. For each pair of variables, the correlations from observed data (columns) and those from the maximum likelihood (ML), generalized least squares (GLS), and asymptotically distribution free (ADF) estimation methods are presented.

| | | Temperature | Colour | Total phosphorus | Chlorophyll *a* | log(Copepods) | log(Cladocerans) |
|---|---|---|---|---|---|---|---|
| Temperature | Observed | 1.000 | | | | | |
| | ML | 1.000 | | | | | |
| | GLS | 1.000 | | | | | |
| | ADF | 1.000 | | | | | |
| Colour | Observed | −0.181 | 1.000 | | | | |
| | ML | 0.000 | 1.000 | | | | |
| | GLS | 0.000 | 1.000 | | | | |
| | ADF | 0.000 | 1.000 | | | | |
| Total phosphorus | Observed | 0.151 | −0.159 | 1.000 | | | |
| | ML | 0.000 | 0.000 | 1.000 | | | |
| | GLS | 0.000 | 0.000 | 1.000 | | | |
| | ADF | 0.000 | 0.000 | 1.000 | | | |
| Chlorophyll *a* | Observed | 0.380 | −0.261 | 0.562 | 1.000 | | |
| | ML | 0.294 | −0.140 | 0.510 | 1.000 | | |
| | GLS | 0.281 | −0.133 | 0.488 | 1.000 | | |
| | ADF | 0.333 | −0.098 | 0.519 | 1.000 | | |
| log(Copepods) | Observed | 0.514 | −0.024 | 0.062 | 0.182 | 1.000 | |
| | ML | 0.513 | 0.000 | 0.000 | 0.135 | 1.000 | |
| | GLS | 0.510 | 0.000 | 0.000 | 0.125 | 1.000 | |
| | ADF | 0.533 | 0.000 | 0.000 | 0.147 | 1.000 | |
| log(Cladocerans) | Observed | 0.719 | −0.201 | 0.179 | 0.288 | 0.505 | 1.000 |
| | ML | 0.714 | 0.000 | 0.000 | 0.188 | 0.481 | 1.000 |
| | GLS | 0.682 | 0.000 | 0.000 | 0.167 | 0.471 | 1.000 |
| | ADF | 0.710 | 0.000 | 0.000 | 0.196 | 0.488 | 1.000 |

expected to be able to include total nitrogen or the different nutrient fractions together with total phosphorus or in place of it under the latent variable 'Nutrients' because Lake Valkea-Kotinen had shown signs of co-limitation of phosphorus and nitrogen during the 1990s (Järvinen 2002, Vuorenmaa et al. 2014), and the dissolved fractions would better reflect the actual interaction between nutrients and phytoplankton. The stepwise multiple regression analysis in Arvola et al. (2014) included phosphate, ammonia, and dissolved inorganic nitrogen together with total nitrogen, total phosphorus, primary production, and colour as explanatory variables for chlorophyll *a*, with adjusted $R^2 = 0.552$. Their results are not directly comparable to ours, however, mostly because their study period was longer (1990–2009), but also because their data included the measurements from a fixed period of weeks 20–39 each year. Thus, although also from the open water period, their data included some occasions when the water column was not stratified. In our trials with different models, total nitrogen seemed to be the least relevant variable, inflating the $\chi^2$ values if it was added. In contrast, the $\chi^2$ values remained low for phosphate and nitrate-nitrite, and the greatest problem in identifying causalities arose from the many values of

**Table 2.** Path coefficients and variances with 4 different estimation methods for the Lake Valkea-Kotinen structural equation model. The estimate for path coefficients is the mean value. Depending on the method, standard errors (SE) together with *p*-values (*p*) or standard deviations (SD) are also given for the estimates. The Bayesian method provided error variances for copepods (ε5), cladocerans (ε4), and total phosphorus (ε3).

| | **Maximum likelihood** | | | **Generalised least squares** | | | **Asymptotically distribution-free** | | | **Bayesian** | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Estimate | SE | *p* | Estimate | SE | *p* | Estimate | SE | *p* | Estimate | SE | SD |
| Cladocerans ← Grazing | 1.954 | 0.262 | <0.001 | 1.770 | 0.232 | <0.001 | 1.789 | 0.192 | <0.001 | 2.022 | 0.002 | 0.325 |
| Phytoplankton ← Colour | −0.197 | 0.096 | 0.040 | −0.196 | 0.102 | 0.054 | −0.165 | 0.106 | 0.118 | −0.195 | 0.000 | 0.098 |
| Phytoplankton ← Grazing | −4.625 | 4.237 | 0.610 | −4.798 | 8.421 | 0.569 | −5.083 | 5.346 | 0.120 | −3.826 | 1.787 | 30.339 |
| Phytoplankton ← Nutrients | 5.736 | 0.753 | <0.001 | 6.054 | 0.765 | <0.001 | 5.433 | 0.555 | <0.001 | 5.844 | 0.006 | 0.846 |
| Phytoplankton ← Temperature | 2.494 | 1.191 | 0.041 | 2.514 | 1.247 | 0.044 | 3.430 | 1.343 | 0.011 | 2.364 | 0.230 | 4.022 |
| Covar(Temperature, Grazing) | 1.793 | 0.320 | <0.001 | 1.711 | 0.304 | <0.001 | 1.875 | 0.218 | <0.001 | 1.851 | 0.002 | 0.350 |
| Var(Grazing) | 0.317 | 0.088 | <0.001 | 0.326 | 0.087 | <0.001 | 0.348 | 0.068 | <0.001 | 0.325 | 0.001 | 0.095 |
| Var(Colour) | 272.291 | 32.202 | <0.001 | 238.446 | 30.011 | <0.001 | 190.246 | 24.725 | <0.001 | 282.184 | 0.151 | 34.000 |
| Var(Nutrients) | 14.508 | 4.195 | <0.001 | 12.709 | 3.591 | <0.001 | 15.866 | 4.191 | <0.001 | 15.336 | 0.022 | 4.455 |
| Var(Temperature) | 13.308 | 1.574 | <0.001 | 12.153 | 1.499 | <0.001 | 13.030 | 1.114 | <0.001 | 13.981 | 0.006 | 1.698 |
| Var(ε5) | | | | | | | | | | 0.617 | 0.003 | 0.181 |
| Var(ε4) | | | | | | | | | | 0.619 | 0.001 | 0.086 |
| Var(ε3) | | | | | | | | | | 34.555 | 0.018 | 4.341 |

those variables that fell under their analytical detection limit during the stratified period. A similar situation for phosphate was reported for Lake Washington data (Arhonditsis et al. 2006), and more frequent measurements or higher *n* for values above the detection limit would be needed to catch some of the interplay between phosphate and chlorophyll *a*. Arvola et al. (2014), with the notably larger dataset from 1990–2009 ($n = 332$), still reported the correlation coefficient between chlorophyll *a* and phosphate in Lake Valkea-Kotinen to be $r = 0.544$ and nonsignificant between chlorophyll *a* and nitrate. Another process that could interfere with the interaction between epilimnetic nutrients and phytoplankton is the ability of some flagellate taxa, like cryptophytes and *Gonyostomum semen*, to migrate between the epilimnion and hypolimnion to access additional nutrients in deeper water (Salonen et al. 1984, Salonen and Rosenberg 2000).

Although we used SEM mostly as a confirmatory tool, one promising feature of SEM was the possibility to explore different model options and test the effect of inclusion or exclusion of some variables on the model outputs. As seen from the standard deviations of the posterior distributions (Table 2), the effect of grazing on phytoplankton was the most uncertain and varied on a wide scale above and below zero. In earlier studies (Arvola et al. 2014, Lehtovaara et. al. 2014) and also in the regression analysis here, the interplay between phytoplankton and zooplankton remained unclear, perhaps because it is not straightforward and not easily detected by traditional methods. During the model building phase, when the included variables changed and different datasets were used (e.g., from summer and autumn months separately), the effect of grazing could occasionally turn positive, which also occurred with copepods in the regression model. Yet Bayesian analysis showed there was actually multimodality in the posterior distribution, with the positive effect eventually gaining the higher peak (maximum likelihood). This finding is somewhat contradictory to conventional views, and although only a side product of the modelling, it raises interesting questions about the phytoplankton–zooplankton relationship in this lake. The presence of *G. semen* may, at least partly, explain the weak relation between phytoplankton and grazing in the final model as well as suggest a counterintuitive positive relation in the trials. *G. semen* is often abundant in Lake Valkea-Kotinen during the late summer; during 1990–2003 it averaged 48% of the total yearly phytoplankton biomass and during 1991–1994 >95% (Peltomaa et al. 2013). *G. semen* seems to be effectively grazed only by some large cladocerans, whereas copepods are not able to control its abundance (Lebret et al. 2012). Stable isotope analyses have indicated that *G. semen* is hardly grazed in Lake Valkea Kotinen (Jones et al. 1999), and thus the effect of zooplankton on *G. semen* may be negligible or may even further boost its growth by eliminating the competing species and recycling nutrients, as demonstrated by Bergquist and Carpenter (1986) and Elser and Goldman (1991). The different sampling technique for zooplankton compared to other variables could also have an effect, however, even though the zooplankton abundance in the whole 5 m water layer probably reflected mostly that in the epilimnion (Lehtovaara et al. 2014).

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**Table 3.** $\chi^2$-test values, degrees of freedom (df), and $p$-values for the Lake Valkea-Kotinen structural equation model with different estimation techniques before (B) and after (A) utilizing error variances gained from Bayesian analyse for copepods, cladocerans, and total phosphorus.

| | **Maximum likelihood** | | **Generalized least squares** | | **Asymptotically distribution-free** | |
|---|---|---|---|---|---|---|
| | B | A | B | A | B | A |
| $\chi^2$ | 15.430 | 16.018 | 11.564 | 13.786 | 15.175 | 15.384 |
| df | 8 | 11 | 8 | 11 | 8 | 11 |
| $p$ | 0.051 | 0.140 | 0.172 | 0.245 | 0.056 | 0.166 |

**Table 4.** Unstandardized (β1) and standardized (β2) regression coefficients with standard errors (SE) given for the unstandardized coefficients and t-test (t) and $p$-values ($p$) for the chosen indicators of chlorophyll $a$ in Lake Valkea-Kotinen.

| | $\beta 1$ | SE | $\beta 2$ | t | $p$ |
|---|---|---|---|---|---|
| Constant | −17.355 | 16.646 | | −1.043 | 0.299 |
| Total Phosphorus | 1.757 | 0.231 | 0.503 | 7.596 | 0.000 |
| Temperature | 2.108 | 0.636 | 0.319 | 3.313 | 0.001 |
| Colour | −0.199 | 0.098 | −0.136 | −2.035 | 0.044 |
| log(Cladocerans) | −1.205 | 1.738 | −0.067 | −0.693 | 0.489 |
| log(Copepods) | 0.429 | 1.980 | 0.017 | 0.217 | 0.829 |

In addition to cladocerans and copepods, there are also protozoans and rotifers present in the lake that were not included in the model. The rotifer data are available, but the principal component analysis showed that they did not group with the other zooplankton; there was a clear seasonal pattern in the highest densities of each group, with those of rotifers and cladocerans clearly diverging (Lehtovaara et al. 2014). Thus, the latent variable "Grazing" is not as straight forward as the measured colour values, and we are missing information about the true grazing pressure, a problem not even the inclusion of latent variables can solve.

The negative effect of colour clearly outweighed that of grazing, and a negative correlation between colour and phytoplankton biomass was also found in Lake Valkea-Kotinen during 1990–2004 (Peltomaa et al. 2013). While higher water colour reduces light availability for photosynthesis, its effect on the shallow epilimnion of Lake Valkea-Kotinen may not be as clear as the model implies (Jennings et al. 2010 and references). Seasonal variation in the colour values tends to be lowest during the summer months (Arvola et al. 2014), when the transport of organic matter from the catchment is low and the water column is stable. Hence, although brown water colour constrains primary production (Carpenter et al. 1998, Arvola et al. 2014), some caution should be exercised when interpreting the model outputs quantitatively because the matching seasonality between colour and phytoplankton may partly explain the higher biomass of phytoplankton during decreasing colour values.

The questions that emerged regarding grazing as well as many of the other interactions could be better addressed with species-level phytoplankton data. The role of one species, *G. semen*, seems to be especially important, and therefore it would be useful to know more about its ecological constraints and effects. Some of the detailed interactions during the growing season are obscured when modelling only total chlorophyll $a$, and even the impact of water temperature varies between species (Reynolds 2006, apparent also in Lake Valkea-Kotinen; Peltomaa et al. 2013). Regardless of these issues, we propose that the SEM presented here provides supporting information for the long-term research at Lake Valkea-Kotinen and is a powerful method to analyse ecological data and, in particular, their complex interactions. Compared to other methods like linear regression, SEM is perhaps more difficult to adopt, yet its better suitability for empirical data, highlighted earlier, is a clear benefit. In addition to the problematic assumptions, many of the methods are unable to describe the system as a network of causalities, thus eliminating their use for detailed predictions about the dynamics of the system. Moreover, linear regression, which is perhaps the most widely used method for describing the relationship between variables (which usually are not linear in nature), should only be used for predictions within the upper and lower limits of the original dataset. Extrapolating to drastically different conditions is thus inadvisable and potentially restricting. This problem can be overcome with Bayesian SEM by using prior information, but if SEM is to be used for predictions it must be tested with an independent dataset from the lake. We also note that the SEM strategy of comparing alternative models to assess relative model fit makes it more robust than regression, which can be highly susceptible to interpretation error due to misspecification (Garson 2012).

A high data requirement has previously restricted SEM studies, but the dilemma of missing data can (to some extent) be eased by utilizing the Bayesian modelling framework. Bayesian modelling also allows us to take the Lake Valkea-Kotinen SEM as a starting point, as prior information, for studies of other lakes. Especially when applying models for lakes with limited available data (e.g., to support lake management), we should aim to evaluate and develop modelling methods that would be flexible and simple to apply regardless of data availability. In future studies, however, a comparison between modelling coarse and detailed data should be conducted to further assess the utility of SEM for less-studied lakes as well as to estimate the minimum data needed for an acceptable model.

In conclusion, SEM for Lake Valkea-Kotinen showed that during summer stratification, nutrients and temperature enhanced phytoplankton growth in a dystrophic lake, whereas high water colour was a significant restricting factor. The effect of zooplankton grazing on phytoplankton was also negative, yet weak. We were able to explore the phytoplankton zooplankton interaction in more detail using Bayesian SEM, which provided new insights about variable interactions in a dystrophic lake and supporting information for the long-term research at Lake Valkea-Kotinen. Considering the many beneficial features of SEM for analysing monitoring data, we encourage its further applications in aquatic science.

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V

# ALTERNATIVE APPROACHES TO MODELLING LAKE ECOSYSTEMS

by

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Article

# Alternative approaches to modelling lake ecosystems

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## Abstract

The development of modelling in aquatic ecology has focused on mechanistic biogeochemical models. However, such models have substantial data requirements for inputs and also for proper validation, which hinders their use for less studied systems. Another significant problem with complex models is their structural and computational difficulty, and thus often an associated absence of proper uncertainty analysis for the model results. This makes the use of the outputs for public policy making (e.g. in lake management) rather questionable. We see no compelling reason (other than lack of awareness of choices) why all lakes and all questions should necessarily be studied using the same high-profile models. Here we review two alternative statistical approaches, Linear Mixed Modelling and Structural Equation Modelling, and the different ways they have been used to extract maximum information from existing data. These methods offer promise for tackling the problems highlighted above, although our aim is not to promote any one method over the others. Rather, we want to stimulate debate about the remaining unknown factors in lake modelling as well as about the balance between data and models, and the still too uncritical way in which model outputs are interpreted and used for decision making.

Keywords: Chlorophyll *a*; lake management; phytoplankton; statistical modelling; uncertainty.

## Introduction

With ecological modelling there is a need to consider carefully, not only the theoretical validity of the model equations, but also their reliability and consistency in describing biological systems. Arhonditsis & Brett (2004) showed through meta-analysis that the performance of mechanistic aquatic biogeochemical models declines the more they shift from physical and chemical processes to biological components of planktonic systems. Also, when the models are used for forecasting or as baselines to study new systems, there is a need to consider very carefully the uncertainty in the model outputs and the information they are actually yielding (Clark et al., 2001).

In this review we do not intend to go deeper into the purely scientific aspects of how modelling should face these questions. Rather, we wish to consider how, from a more practical and basic standpoint, these issues

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affect application of models in lake management. At present, attention seems to be focused on further and joint-development of the (strongest) existing mechanistic biogeochemical models, with very detailed descriptions of the aquatic system (see Jørgensen, 2010; Mooij et al., 2010; Trolle et al., 2012). Although the development of these models has been intense during recent decades and many methodological improvements have been achieved (see Jørgensen, 2010 for a short review), it is not clear that the problems highlighted above are overcome when applying the models to study new interactions outside their base equations and the environment into which they are fixed (Rykiel, 1996). For this reason, the most apparent drawback with applying process-based biogeochemical models for management purposes (besides expensive licenses, high computational costs and complexity) is that they require a substantial quantity of both detailed data for input and independent data for validation.

This means that for a lake that has not been well studied, the credibility of the model and its function in the new system may become impossible to judge and its validity cannot be confirmed (discussed by Oreskes et al., 1994; Rykiel, 1996; Arhonditsis & Brett, 2004). Indeed, this is often the situation when utilising models in lake management, even though the predictive power of models during the decision-making process would then be crucial. For example, many of the lakes covered by the EU Water Framework Directive (European Parliament & Council, 2000), that presents water quality requirements, have not been studied sufficiently intensively to permit good quality process-based modelling. One solution could be to apply less complex models for less studied systems. However, in many cases the simple equations are not sufficient for the questions of interest and for exploring the system function. The right time and space scale is crucial for addressing more detailed questions, and the often averaged predictions of simple models can only offer insight into large-scale processes.

Statistical methods have received surprisingly little attention in ecological, and especially in aquatic modelling (Arhonditsis et al., 2006; Kruk & Segura, 2012), even though they could offer more efficient and reasonable ways to exploit sparse data. An even stronger reason to think that statistical methods can represent a good option is the possibility for sufficient uncertainty analysis. Even when provided with ostensibly sufficient data, the interactions among different variables in open systems are neither clear nor stable, so that the possibilities to make accurate measurements of everything essential are limited (Oreskes et al., 1994). Yet proper evaluation of the predictive accuracy of mechanical models has received too little attention, probably because when the very detailed models inevitably become very complex the task becomes extremely difficult (Robson et al., 2008; Doherty & Christensen, 2011). This has raised particular criticism of the use of biogeochemical models as a basis for public policy decisions (Oreskes et al., 1994; Malve, 2007; Ramin et al., 2012). Similarly, the scientific value of the model outputs can be difficult to judge if no uncertainty analysis is performed, Arhonditsis & Brett (2004) reporting on the lack of uncertainty analyses in 153 modelling studies undertaken between 1990 and 2002.

However, with most commonly used statistical methods, we soon face the (often ignored) problem that data or model residuals do not meet the assumptions of either normality or homogeneity, fixed explanatory variables, independence of observations or a correct model specification (Zuur et al., 2009). Using the methods *anyway* or not understanding the true meaning of the assumptions can in the worst case lead to false models and false interpretations of the system. Especially with observational data, problems arise with traditional linear models (and regressions) as one of their essential features is to assume only the dependent variable to be subject to measurement error or other uncontrolled variation. With ecological field data, this is not achieved (Zuur et al., 2010). Thus, there is a need to identify novel methods that do not have, or can handle, the non-fulfilment of those assumptions, because if we seek to learn about causal relationships in nature we cannot rely only on controlled experiments (Shipley, 2002).

Here we consider two methods, linear mixed modelling (LMM) and structural equation modelling (SEM), to promote the idea that instead of concentrating too much on developing all-embracing models we should constantly

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seek new and adequate modelling tools to extract the most ecological information from the available data, while at the same time acknowledging the unpredictability and multi-dimensionality of nature, that may be simply impossible to compress into equations. It is crucial to recognise the stochasticity of nature and handle it in the right way (Clark et al., 2001), as well as to bear in mind the heuristic nature of models (Oreskes et al., 1994; Otto & Day, 2007).

Both LMM and SEM appear to represent interesting alternatives for studies with environmental data, although at present their ecological applications, especially for aquatic environments, are still growing. The reasons these methods have not been used more in general have mostly been inadequate computing power and lack of freely available software (Zuur et al., 2010). In addition, these methods are of course more complicated to adopt than some more common statistical methods (Zuur et al., 2009). In the case of path analysis, from which SEM is derived, and the original work of geneticist Sewall Wright, it was also not able to compete with Fisher's methods at the beginning of the 20th century and was ignored (Shipley, 2002).

We will introduce the use of LMM and SEM for phytoplankton- and eutrophication-related studies of lakes and summarise their benefits compared to more customary methods. Although there are several other methods, these two were selected because they:

- have interesting, novel approaches to study ecological questions;
- are relatively easy to adopt with the help of some statistical support;
- do not require extensive input data;
- are executable using normal computing power;
- already have some published applications for aquatic environments, including phytoplankton, for comparison;
- can be applied with free software like R (R development core team, 2012).

In addition, they can be combined with Bayesian inference. In the Bayesian mode of thinking, external information outside the observed dataset can also be used in the analysis. Assimilating this so-called prior information from earlier studies or literature helps to utilise all the available information about the phenomenon. Moreover, any new information gained afterwards can easily be added into the model. In Bayesian inference, model parameters are considered as random variables and they are assigned a probability distribution (Ellison, 2004). In environmental decision making, the Bayesian approach is appealing, as the uncertainty and error in data and in the predictions can be statistically quantified and considered. One limitation of Bayesian analyses has been its computational difficulties and thus greater requirement for computing power. However, this problem is overcome with the help of modern computing software. A thorough and mathematically emphasised introduction to Bayesian data analysis can be found in Gelman et al. (2003) and a more practical introduction for ecologists in Ellison (2004) and Clark (2005).

## Linear Mixed Modelling and Structural Equation Modelling in phytoplankton studies

We undertook a search in the Web of Science (http://thomsonreuters.com/web-of-science) concentrating on those articles that actually introduced an application for phytoplankton and perhaps linked this to eutrophication problems. Because the selected statistical methods can be referred to by different terms, for structural equation modelling we conducted the search with: ('phytoplankton' OR 'chlorophyll') AND ('structural equation model*' OR 'causal model*' OR 'latent variable structural equation*' OR 'analysis of covariance structure*') (taken from Rigdon, 1998). For mixed effects models we wanted to include possible non-linear applications and did the search with: ('phytoplankton' OR 'chlorophyll') AND ('hierarchical linear model*' OR 'multilevel model*' OR 'random effects model*' OR 'mixed effects model*' OR 'mixed model*').

For SEM the number of relevant articles was 13 and for LMM seven. We could not access one of the SEM articles (Kenney et al., 2009), but according to its abstract and list of authors it is closely related to some of the other papers. From the 19 papers used for this review, seven used a Bayesian approach. Some additional papers listed in the search had chlorophyll *a* only as a proxy for some other factor and so these were omitted from this review. None of the 19 papers reviewed was published before 2004 and most were quite recent. As a comparison, a query for SEM without the restricting terms phytoplankton and chlorophyll *a* gave over 19 000 papers, most from the field of psychology and a little over 300 falling into the Ecology category. For mixed effects models the total number of papers was over 30 000, of which about 900 were in the Ecology category.

When looking at the number of citations and the citation history of the 19 SEM and LMM papers referred to here, two issues arose. Firstly, the papers have not generally gained many citations, and secondly they are mostly cited in journals like *Ecological Modelling* and *Environmental Modelling and Software*. This indicates that currently they do not really represent the 'mainstream' aquatic modelling that reaches the more common limnology-related journals.

## Mixed effects models

After using linear regression, the step towards linear mixed effects (or hierarchical) modelling (LMM) should not be too difficult, because they have much in common. Besides the *lme* and *gls* packages for R, some basic statistical programs like SPSS (IBM) have a guided function for mixed modelling. The advantages of LMM compared to linear regression arise from its capacity to cope with temporal and spatial correlation and repeated measurements for all types of data. LMM is especially suitable for complicated data structures, like nested or hierarchical data (Zuur et al., 2009). These data structures are common in ecology where the observations are naturally grouped so that the individual samples in the same group are not independent.

In the linear mixed model the response variable is expressed as a linear sum of so-called fixed and random variables (=mixed). The fixed part of the model is usually the 'regression part' and fixed parameters contribute to the overall mean value of the dependent variable, in which we are usually interested. The random part of the model expresses the covariance structure of the data, and we are not interested in the variables as such (see e.g. Clark, 2007). Thus in lake water quality modelling the fixed part could be the main and/or joint effect of nutrients on phytoplankton and the random part the covariance structure of selected variables between and within lakes. Constructing LMM starts by defining the fixed variables of the model, in the same way as for linear regression modelling. By adding random variables one by one (lake effect, lake type effect, etc.) the sufficient covariance structure will be found (see Zuur et al., 2009 for more details).

Besides being linear, mixed effects models can also be additive, depending on the relationships between the variables. Zuur et al. (2009) have given a good example of how to apply additive mixed modelling to phytoplankton time series data that have several complicating factors. They used data for which the environmental variables and phytoplankton variables had sometimes been measured at different times, and containing a large number of phytoplankton species, possible temporal and spatial correlation, as well as heterogeneity and non-linear trends over time. In addition the data were irregularly spaced and the phytoplankton had been counted in different laboratories. The example is a very good introduction and discusses not only the advantages of mixed modelling, but also the emerging problems and possible solutions.

In practice, a hierarchical model structure has proved useful when we want to utilise effectively large datasets (for example from environmental monitoring) in which the number of monitored lakes is large but the number of observations for some individual lakes may be small. Thus, to make predictions for one lake, all pieces of information can be put together by weighting the most relevant (lake-specific) data, but filling the gaps in information with the help of the whole dataset (so-called 'borrowing strength theory'). The selected papers gave examples of how water quality data can be further grouped into intermediate hierarchy levels based on different ecoregions (Lamon & Qian, 2008), landscapes (Wagner et al., 2011) or lake types (Malve & Qian, 2006) to acknowledge the differences and similarities that these features may bring at the lake level to the processes of interest. This demonstrates the advantage over normal regression, as we can acknowledge the effect of, say, lake depth on the phosphorus–chlorophyll *a* relationship (see also Phillips et al., 2008), without having to

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split the big dataset for separate regression, and thus gain a more powerful yet realistic model (Malve & Qian, 2006).

The idea can also be used the other way round, to test into what kind of groups it is reasonable to divide lakes for their assessment, so that the groups actually explain variation in the responses (Cheruvelil et al., 2007). For the intercalibration of ecological data within EU countries, Thackeray et al. (2013) used hierarchical modelling to show that variation within certain proxies for eutrophication (chlorophyll-*a* concentration, Phytoplankton Trophic Index and total cyanobacterial biovolume) was highest at the among-lake level and not among persons handling the samples.

All the above mentioned studies applied LMM, whereas the additive method has been used by Carvalho et al. (2011) when trying to determine risk factors for cyanobacterial blooms. Their modelling showed that at a national scale the lake water colour followed by alkalinity increased the risk. The additive method has also been used to study and acknowledge differences among lakes and years when estimating the effect of nutrient availability and temperature on different phytoplankton groups (Salmaso et al., 2012). Thus, the studies are very similar to those done with LMM, but with the additive method allowing non-linear relationships between variables.

In three of the papers (Malve & Qian, 2006; Lamon & Qian, 2008; Wagner et al., 2011), Bayesian inference has been included into the modelling. Lamon & Qian (2008) stated that, because of problematic data, the Bayesian method was essential for their model estimates. When the number of hierarchy levels and the number of model parameters grow, the parameter estimation becomes difficult due to complex equations. Thus, obtaining analytical or closed-form solutions to them becomes impossible, leaving the Bayesian sampling-based approach as the only option (Clark, 2007). Actually it is more a rule than an exception that Bayesian inference is used in the mixed effects model analysis. On the other hand, the term 'fixed effects' in the Bayesian context is a bit confusing, as all the parameters are random (Gelman et al., 2003). Therefore, it is more common to use the term hierarchical Bayes, whenever there is a mixed/multilevel modelling and a Bayesian approach is involved. From a more practical point of view, the posterior distributions from Bayesian analysis give a more tangible idea of the uncertainty in estimates (Malve & Qian, 2006).

LMM and additive modelling seem to be efficient tools to make the most of sparse monitoring data, and, on the other hand, to make deductions that take into account the natural variation between sites. Malve & Qian (2006) showed how the hierarchical model fit for three different lakes was better than that of a non-hierarchical lake type specific model. However, sometimes the preciseness of the hierarchical levels may not be clear. For instance, there has been debate (Lamon et al., 2008) about the accuracy of dividing Finnish lakes into the different types that are used in Malve & Qian (2006), whereas Wagner et al. (2011) point out that they had to make a lot of assumptions with the landscape data. Of course, the selected hierarchy may not always highlight any notable differences; for example, the growth of some phytoplankton species may be more consistent among different lakes than that of others (Salmaso et al., 2012).

## Structural equation modelling

Structural equation modelling (SEM) is a component of applied multivariate statistical analyses that emphasises causal effects through the study of path relations. It is not directly a statistical technique but a scientific framework within which new techniques can be added as they become available (Grace et al., 2010). Essentially SEM is an extension of the general linear model, but a rather deeper introduction to SEM than to LMM is probably needed, and a thorough explanation of the different steps of SEM can be found from Shipley (2002). Nevertheless, using SEM programs does not actually require a very detailed understanding. R has packages for SEM, but it may be easier first to adopt the technique using some of the commercial packages, which are more visual. Some free student versions are available, for instance SPSS AMOS (IBM), but unfortunately that does not include the Bayes function.

Unlike for linear regression, in SEM it is possible to include multiple dependent variables and hence to obtain a better overall picture of the system function. SEM can also handle difficult data, like time series with auto correlation as well as non-normal or incomplete data. One useful property for ecosystem studies that distinguishes SEM from simple path models is the inclusion of latent variables (Shipley, 2002). A latent variable is one that cannot be measured directly, and hence it can be more hypothetical and theoretical (Hershberger et al., 2003). However, it is usually more convenient and justifiable to include a latent variable if it can still be observed through directly measurable variables that are linearly related to it (Shipley, 2002). The inclusion of latent variables also allows us to capture the unreliably of measurement in the model. For instance, we can measure some nutrient fractions from the water, but since we know they do not explain the growth of phytoplankton directly as such, we create a latent variable 'nutrients' (see e.g. Fig. 4 in Arhonditsis et al., 2006 for illustrative example).

SEM can be used either to confirm a theory by testing it against empirical data or to explore the potential relationships between different variables and build up theories (Hershberger et al., 2003). Especially when building up theories it is necessary to consider very carefully what is the quality and the representativeness of the data. The first step in SEM is to establish a conceptual model and a path diagram of the interactions between different variables and to form a framework for model development (this is why using R instead of the commercial packages may feel difficult at first, because with them the model building starts simply by drawing the variables and paths between them, which is not possible in R). Besides literature, principal component analysis (Chou et al., 2012) and/or linear regressions (Liu et al., 2010) can be used to identify the major sources of influence on responsible variables, before constructing SEM.

Of the 12 articles we selected, half introduce SEM for studying the effect of nutrients and other ambient factors on chlorophyll-*a* concentrations and phytoplankton biomass but also on different phytoplankton groups within the community (Arhonditsis et al., 2006, 2007a, b; Liu et al., 2010; Salmaso, 2011; Gudimov et al., 2012). One climatic-change-related review uses SEM as part of the analysis to elucidate some of the key causal relationships that affect the interplay between different variables and phytoplankton (Shimoda et al., 2011). The planktonic food web and prey–predator interactions are studied in one of the articles (Shinada et al., 2005), and four articles focus on biodiversity, often also including a regional or latitudinal effect (Korhonen et al., 2011; Stomp et al., 2011; Chou et al., 2012; Matthews & Pomati, 2012).

After establishing the conceptual model, estimates for the paths (parameters) are calculated with the help of maximum likelihood estimation or weighted least squares, so that the model is able to create a variance-covariance (or correlation) matrix for the variables, congruent to the one observed (see Hershberger et al., 2003). A key element in model building is that inclusion or exclusion of a pathway should be based on theoretical justifications instead of being an automatic procedure. In addition, the pathways should be kept to a minimum and the model as simple as possible (Grace et al., 2010). Indeed, SEM with too many interacting variables becomes onerous to interpret and follow (as in Stomp et al., 2011).

The null hypothesis in SEM is that the observed covariance matrix equals the model-implied one and that the model can be accepted. Hence, a very important feature for the interpretation of results is that the aim is the acceptance of $H_0$, not rejection. For instance $X^2$-test can be used to test the congruity between the observed and modelled matrices. The value of $X^2$ should be as small as possible, degrees of freedom should be high and $p$ higher than 0.05 (see e.g. Shipley, 2002; Hershberger et al., 2003; Grace et al., 2010). There are also other options that can be used instead of or together with the $X^2$-test, like the root mean square error of approximation (RMSEA) and the goodness of fit index (GIF) (used in Shinada et al., 2005; Arhonditsis et al., 2007a; Chou et al., 2012).

When the best possible model is identified, the direct paths between different variables can be examined to see the direction and strength of their interactions. The (usually) standardised path coefficients between variables are equivalent to the slopes in normal regression. However, when latent variables are included, the total standardised effect of measured variables on

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the dependent variable is calculated by multiplying the effect between the measured and latent variables and that between the latent and dependent variables.

Interestingly, the studies selected show that physical factors, especially temperature, more consistently influenced phytoplankton growth and dynamics (e.g. Arhonditsis et al., 2007a; Chou et al., 2012), although the influence was not uniform between different places (Arhonditsis et al., 2007b). The role of nutrients varied and the addition of some key growth element such as phosphate (if comparing Arhonditsis et al., 2007a and b) did not markedly improve the model. As Arhonditsis et al. (2006) pointed out, in phosphorus-limited environments the normal monitoring sampling frequency is too low for detecting the actual relationship between phytoplankton and phosphate concentrations, the latter usually falling under detection limits. Models that included separate phytoplankton groups instead of total chlorophyll *a* seemed to be more efficient in elucidating the more detailed interactions, such as between temperature, nutrients, zooplankton and phytoplankton (Arhonditsis et al., 2006; Shimoda et al., 2011).

The interpretation of SEM results is perhaps the most critical part, especially when latent variables are present. Some of the articles were confusing to read, when for instance SEM with $X^2 = 183.9$ and $p < 0.01$ (no degrees of freedom given, Matthews & Pomati, 2012) was reported to be the best model. Also, there was some incoherence in interpreting the results. In Liu et al. (2010) the latent variable 'toxic substances' was included in the model and some of the substances were argued to have a relatively large effect on phytoplankton. However, the total standardised effects of cyanide, arsenic, cadmium and fluoride can be calculated to be (-0.0022) to (-0.0001), which does not support the authors' interpretation.

Besides illustrative introductions to applying SEM correctly in ecological studies (Shipley, 2002; Hershberger at al., 2003; Grace et al., 2010), there are good papers discussing how to incorporate results from SEM studies into research papers (Hoyle & Panter, 1995; Boomsma, 2000). With methods like this that can be applied in many different ways it is crucial not to confuse the reader or omit any information that enables the logic of modelling to be followed and the right interpretation of the results. With the freedom that is mentioned as one of the appealing features of SEM (Arhonditsis et al., 2006), there also comes responsibility.

There were four studies that combined Bayesian inference with SEM (Arhonditsis et al., 2006, 2007a, b; Gudimov et al., 2012). One of them (Gudimov et al., 2012) used Bayesian networks, which enables assessment of the uncertainty in the final result when integrating various models (with uncertainties) into one framework. The biggest advance in including the Bayesian approach, especially with SEM, is that it does not rely on asymptotic theory, thus allowing smaller sample sizes (Arhonditsis et al., 2006). As the inferential tests of SEM are otherwise asymptotic, the required sample size is high (Shipley, 2002). Some extra information can also be gained compared to the maximum likelihood method, if there is more than one local maximum for describing the phenomena.

## Concluding remarks

LMM and SEM are both illustrative and interesting tools to explore aquatic environments. With both methods some new ideas about the interactions between different variables and phytoplankton are highlighted in published studies. For this reason – the possibility of deriving 'hints' of underlying processes, even of those not directly observable (Malaeb et al., 2000), which can then be used in developing further ideas and studies – ecological modelling with different techniques should be encouraged (Oreskes et al., 1994). There should be more space for exploration and creativeness when using models as a tool, instead of the idea that we should aim for a 'perfect' model, capable of describing the system as we see it.

Yet we emphasise that the techniques reviewed here are by no means the only ones, or necessarily the most suitable for addressing every question. There are some notable differences even with LMM and SEM, as LMM seem to be more suitable for refining information from sparse, big datasets, whereas SEM can more readily elucidate the patterns within systems. It is perhaps easier to understand how LMM (like regression) can be utilised in lake management and predictions, but for SEM there is also a good demonstration in Arhonditsis et al. (2006). Although it puts one outside of 'the comfort lines', whether the customary model is the best one to be used for new kinds of questions should always be considered. No one is capable of mastering all the techniques, which strengthens the case for interdisciplinary cooperation.

Whatever the technique, it is important to keep in mind that, although the theory behind the statistical models is fixed, there is always, as in any kind of modelling, some degree of subjectivity involved when determining the interactions between different variables and setting up models. Because the models can be built up in many different ways, there needs to be enough information in the publications for anyone interested to repeat the modelling process to judge its logic (Hoyle & Panter, 1995; Boomsma, 2000). This is especially true when introducing novel methods. However, since free software for statistical modelling is available, and the calculations are done through standard statistical equations, the methods are actually, at their best, very transparent ways for using models in science.

As discussed earlier, proper uncertainty analysis should be customary in ecological modelling, especially when used as a basis for public policy making. In fact, not all LMM and SEM papers referred to here considered the uncertainty adequately. If any, the 95 % confidence intervals or similar were most used for model outputs (Malve & Qian, 2006; Arhonditsis et al., 2007a, b; Wagner et al., 2011; Gudimov et al., 2012) and some papers including Bayesian analysis introduced few posterior distributions for the estimates (Arhonditsis et al., 2006; Gudimov et al., 2012). The benefit of proper uncertainty analysis is not just in the awareness and in the possibility to evaluate the model performance. In situations when the uncertainty in model results for management planning becomes unacceptable, they can still be used to indicate where future monitoring efforts should be targeted to decrease the uncertainty (Lamon & Qian, 2008).

Related to this, there should in general be some consideration of the minimum amount of data that is needed to do any kind of modelling for a study lake, especially if we go into more detailed questions about eutrophication or phytoplankton. In management projects, models are unfortunately sometimes seen as a substitute for sampling. Otto & Day (2007) framed this very concisely: *'- - - But without data, collected in the field or in the lab, mathematical models can never tell us what has happened or what is happening. Thus, it would be foolish to promote mathematical biology above other areas in biology.'* Even with adequate sample sizes, but too long sampling intervals, SEM was not able to catch all the interesting interactions. Another issue is the importance of sampling done after modelling, to verify the model results and see if they hold.

Besides these questions about proper modelling technique and data, we agree with Ramin (2013) that more critical evaluation of the limits of modelling is needed. Our trust in models is sometimes too great, although there are still many indisputable unknown factors. A good example is how many current modelling studies aim to illustrate the effects of climate change. While the question is of high importance, the use of models to predict the future from certain offsets and assumptions is in the worst case highly misleading. The predictive power of models decreases fast the further the simulation proceeds from the starting point, especially with phytoplankton (Arhonditsis & Brett, 2004; Benincà et al., 2008). In addition, the environment for which we now calibrate the models will not be the same in a hundred years, which challenges the credibility of the predictions (see Rykiel, 1996; Clark et al., 2001). As a more concrete point of comparison with aquatic modelling, one can consider the long tradition of meteorological studies and modelling, and the accuracy of weather forecasts for the coming weekend!

The validity of the model results is of course also a matter of the scale of modelling, with the bigger, more average processes being easier to 'capture'. However, then the information content (see Clark et al., 2001) of model outputs suffers, and in a way they become 'predictable'. Instead of putting high effort to 'confirm' what is already known (which is often done through calibration and really ignores the true cause of results), should we instead be more committed to preventing these possible scenarios


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from taking place, and at the same time focus the modelling effort towards exploring the unknown? Of course, any development and progress needs these kinds of first steps, but whether the present way of modelling is justifiable for management and public policy making should be evaluated very carefully. That it 'saves money' is often the strongest, but very unfortunate justification. Without proper uncertainty analysis it can even be a false one.

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## Author Profile

During the past four years, as her still on-going PhD work, M.Sc. **Anita Pätynen** has been testing different kinds of models and techniques, e.g. PROTECH, Structural Equation Modelling and MyLake, to find out how well they can be applied with Finnish lake data, and what are the challenges when putting together the often sparse monitoring data (with strong seasonal variation) and model applications. Already for her Master's diploma work (Aquatic Sciences, University of Jyväskylä, 2009), Pätynen tested and took part in developing the Lake Load Response model tool at the Finnish Environment Institute, that is developed to ease the use of models in lake management. She has been actively involved in the lake management and Water Framework Directive related work at the Modelling and Assessment unit of the Finnish Environment Institute since the start of her Master's diploma work at 2008.

M.Sc. **Niina Kotamäki** (Finnish Environment Institute SYKE) is a statistician whose expertise is in applying sophisticated statistical methods in water quality modelling e.g. hierarchical Bayesian and structural equation modelling. She has been developing and using statistical and process-based phytoplankton models in lake ecosystems.

**Dr Olli Malve** has enthusiastically pursued methods for predicting and managing hydrological, chemical and biological processes in surface waters and achieved exceptional experience in modelling complex systems. The problem of decision making under uncertainty has inspired him to explore combinations of mechanistic and statistical methods using Bayesian inference and MCMC sampling methods. To accomplish this and to apply the developed methods in river basin management he has collaborated with many statisticians, mathematicians, biologists and environmental managers. As the editor of the scientific journal Aqua Fennica and as a lecturer he has participated knowledge transfer activities on his field. Recently, he has managed lake and river modelling team in Finnish Environment Institute.

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