Estimating the critical phosphorus loading of shallow lakes with the ecosystem model PCLake: Sensitivity, calibration and uncertainty

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ABSTRACT

There is a vast body of knowledge that eutrophication of lakes may cause algal blooms. Among lakes, shallow lakes are peculiar systems in that they typically can be in one of two contrasting (equilibrium) states that are self-stabilizing: a 'clear' state with submerged macrophytes or a 'turbid' state dominated by phytoplankton. Eutrophication may cause a switch from the clear to the turbid state, if the P loading exceeds a critical value. The ecological processes governing this switch are covered by the ecosystem model *PCLake*, a dynamic model of nutrient cycling and the biota in shallow lakes. Here we present an extensive analysis of the model, using a three-step procedure. (1) A sensitivity analysis revealed the key parameters for the model output. (2) These parameters were calibrated on the combined data on total phosphorus, chlorophyll-*a*, macrophytes cover and Secchi depth in over 40 lakes. This was done by a Bayesian procedure, giving a weight to each parameter setting based on its likelihood. (3) These weights were used for an uncertainty analysis, applied to the switchpoints (critical phosphorus loading levels) calculated by the model. The model was most sensitive to changes in water depth, P and N loading, retention time and lake size as external input factors, and to zooplankton growth rate, settling rates and maximum growth rates of phytoplankton and macrophytes as process parameters. The results for the 'best run' showed an acceptable agreement between model and data and classified nearly all lakes to which the model was applied correctly as either 'clear' (macrophyte-dominated) or 'turbid' (phytoplankton-dominated). The critical loading levels for a standard lake showed about a factor two uncertainty due to the variation in the posterior parameter distribution. This study calculates in one coherent analysis uncertainties in critical phosphorus loading, a parameter that is of great importance to water quality managers.

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1. Introduction

1.1. Eutrophication of lakes

Eutrophication of lakes and other surface waters is a worldwide problem (e.g. Smith et al., 1999). Some 40 years of study have led to increasing insight in the response of lake ecosystems to nutrient loading, starting with the pioneering work of Schindler (1974, 1977) on phosphorus as limiting nutrient for algal crop, and Sakamoto (1966) and Vollenweider (1968, 1975, 1982) on TP and chlorophyll models. These steady-state models were the first to use the mass balance approach to lakes. Several modifications were made to the Vollenweider model (e.g. Dillon and Rigler, 1974; Kirchner and Dillon, 1975; Jones and Bachmann, 1976; Larsen and Mercier, 1976; Reckhow, 1979; Canfield and Bachmann, 1981; and

others; see e.g. Reckhow and Chapra (1983) and Harper (1992) for overviews). All these models allowed to derive average nutrient and chlorophyll concentrations (and sometimes transparency) to P and N loading and some basic lake features of which mean depth and retention time proved to be the most important. Loading criteria, together with uncertainty bounds (Reckhow and Chapra, 1983), were derived for the classification of lakes in different trophic states (ultra-oligotrophic, oligotrophic, mesotrophic, eutrophic or hypertrophic). These states could be defined both in terms of TP, TN and chlorophyll concentrations, in terms of transparency and also in terms of characteristic species composition. Because of the limitations of static models, a.o. to predict response times to management measures and to account for the role of sediments and, later, also food web effects (e.g. Carpenter et al., 1985), dynamic models for TP and chlorophyll were developed (see overviews by Chapra and Reckhow (1983), Jørgensen (1995), Jørgensen et al. (1995), Jørgensen and Bendoricchio (2001), among others). All these models were made for more or less deep, phytoplankton-dominated lakes. Data on shallow lakes (up to several metres)

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revealed that nutrient dynamics is strongly influenced by the presence of macrophytes in these lakes (e.g. Scheffer, 1998; Jeppesen et al., 1998), as they constitute an additional pool (permanent or seasonal) for retention of nutrients and an additional link between water column and sediment. Hence, macrophyte-dominated lakes can have a high transparency and a low chlorophyll level despite a rather high nutrient loading (whereas in the traditional models, shallow lakes would end up almost inevitably as (hyper)eutrophic regardless of their loading). A high transparency is also is a key factor for the survival of submerged macrophytes (e.g. Spence, 1982; Chambers and Kalff, 1985; Jeppesen et al., 1998); hence it can be both cause and result of macrophyte dominance. These mutual relationships, besides other mechanisms, lead to the often observed non-linear behaviour of shallow lakes (Scheffer, 1998). Shallow lakes typically can be in one of two contrasting (equilibrium) states: a clear state with submerged macrophytes or a turbid state dominated by phytoplankton. Eutrophication by excess input of nutrients (phosphorus and nitrogen) may cause a switch from the clear to the turbid state, if the nutrient loading exceeds a critical value (e.g. Carpenter et al., 1992; Scheffer et al., 1993; Gunderson and Pritchard, 2002). This is generally considered as undesirable, because natural communities characterized by macrophytes and a rich fish fauna disappear and biodiversity decreases. Recovery of the clear state is difficult, as the critical loading for the switch back is often lower (hysteresis). A system of interacting ecological processes makes both states stabilize themselves (Scheffer, 1998).

These phenomena were studied extensively by means of 'minimal models' (Scheffer, 1998), but few models combine both nutrient cycles, phytoplankton and macrophytes in a dynamic way. This is the aim of the model *PCLake* (Janse, 1997, 2005), a dynamic model of nutrient cycling and biota (including phytoplankton, macrophytes and a simplified food web) in shallow lakes. The objectives of this model are to estimate the critical nutrient loading levels for this switch, both 'forward' and 'backward', to determine how these levels depend on lake features and management factors, and to identify the key processes determining the switch.

Janse et al. (2008) showed that the model can indeed be used to estimate these threshold values, and concluded that the critical loading levels depend, among others, on the water depth, lake area, retention time, type of sediment and relative area of marsh zone. The present paper concentrates on the model calibration and on the estimation of the uncertainty in the predictions due to parameter variations.

1.2. Uncertainty

Although ecosystem models are often useful tools for the study of environmental problems, they contain a great deal of uncertainty, coming from different sources (e.g. Chapra and Reckhow, 1983; Van Straten, 1986; Somlyódi and Van Straten, 1986; Beck, 1987; Hilborn and Mangel, 1997; De Blois, 2000; Jørgensen and Bendoricchio, 2001). (a) Some of the uncertainty lies in the model structure itself, as we do not know whether the model is a correct representation (in view of the objectives of the model) of the system studied. Several possible model structures might be an equally good representation of the system. (b) Another source of uncertainty are the parameter values, which often can only be estimated and/or exhibit an inherent variability because of spatial, temporal and/or species variations. (c) This problem is even enhanced if the model is to be suitable for different situations. (d) Among these parameters are also the initial conditions of the system, which might influence the results in non-linear models. (e) Finally, when model results are compared with measured data, also these data exhibit a certain level of uncertainty. So, we have to do with 'intentional' uncertainty (because of natural variability) and

unintentional uncertainty (because our knowledge of the system is incomplete).

Ecological models thus typically are poorly identifiable systems, and PCLake is no exception. A compromise usually has to be found between 'physicality' (the model structure should be related to the causal mechanisms acting in the system under study) and 'identifiability' (it should be possible to estimate the unknown model parameters from available data) (Reichert and Omlin, 1997; Omlin et al., 2001). PCLake was set up in a way to remain close to the causal relationships in the lake, to meet the objective of applicability in a broad range of external factors (extrapolation). The disadvantage of this is the occurrence of many parameters which are poorly identifiable from an existing, typically limited, data set. Hence, an 'overparameterized' model was preferred over an 'overly simple' model. For this kind of models, the Bayesian approach for parameter estimation and prediction uncertainty is regarded as the most adequate (e.g. Reckhow and Chapra, 1983, p. 51; Klepper, 1997; Reichert and Omlin, 1997; Omlin and Reichert, 1999; Hilborn and Mangel, 1997), for several reasons:

- The Bayesian method can deal with *probability distributions* of parameters (and model structures), in contrast to traditional calibration where one seeks for single-point estimates.
- The method combines in the analysis prior knowledge of parameters and processes with information contained in the data. This prior knowledge replaces to some extent the (non-existing) data outside the domain of the data set.
- The approach directly yields an uncertainty analysis when used as a prediction tool.

Drawbacks of the method are a loss of accuracy, with wider (but probably more realistic) uncertainty bounds, and an increase in computational demands because many model runs are required.

Hence, we adopt the Bayesian way of model evaluation, realizing that model parameters are ill-defined, intrinsically variable entities, rather than well-defined, fixed numbers. The focus in this project is on the model predictions; the parameter values are only of intermediate interest. The main topic is how the parameter uncertainties propagate in the uncertainties of the model results and predictions, which then can be given in a probabilistic way. We follow the method previously outlined by Aldenberg et al. (1995). In brief, the so-called posterior parameter distribution is based on a combination of prior knowledge and the likelihood, a measure for the degree of fit between model and data. The likelihood is used as a weighing factor for each run (parameter combination). The resulting set of predictions is the posterior predictive distribution (which is usually narrower than the prior predictive distribution, i.e. before the calibration). In practice, the weight is based on the sum of squared residuals (differences between simulations and data) as commonly used in regression analysis (Box and Tiao, 1973/1992). The posterior parameter distribution is thus inversely proportional to the sum of squares raised to the power $n/2$, with n the number of observations. For two or more variables, the probability function can be approximated as the product of the sums-of-squares.

Prior to the likelihood calculations, however, a sensitivity analysis is needed as a first step in the model analysis, to determine which parameters have the most influence on the model results. This step is important in order to make a preselection of parameters for calibration. The parameters to focus on are the ones that are both sensitive and uncertain (Van Straten, 1986). The sensitivity analysis can be applied to both the model outputs themselves, and to the likelihood measure (or fit function). The latter set may be smaller than the first one, e.g. a parameter may have great influence in a region with low likelihood (Ratto et al., 2000).

In this paper, the PCLake model is evaluated by a method combining these three steps, viz. sensitivity analysis, calibration and