18th European Symposium on Computer Aided Process Engineering – ESCAPE 18
Bertrand Braunschweig and Xavier Joulia (Editors)

Developing A Lake Eutrophication Model And Determining Biogeochemical Parameters: A Large Scale Parameter Estimation Problem

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Abstract

This work addresses the dynamic parameter estimation problem for an eutrophication model, which is formulated within a simultaneous approach. Ecological processes are modeled through a set of complex nonlinear differential algebraic equations, with rate coefficients that must be estimated. Gradients of state variables are considered along the water column, rendering a partial differential equation problem, which is transformed into a differential algebraic (DAE) one by spatial discretization in several water layers. Within a simultaneous approach, the DAE constrained optimization problem is transformed into a large-scale nonlinear programming problem. Main biochemical and chemical parameters have been obtained, which allow a close representation of the lake dynamics.

Keywords: Parameter estimation, eutrophication model, phytoplankton, nutrients.

1. Introduction

The increasing download of nutrients into lakes, rivers and costal zones throughout the world, mainly due to agricultural and industrial activities, have intensified eutrophication of water bodies, which has in turn increased the need for predictive ecological water quality modeling. Eutrophication models provide a representation of major physical, chemical and biological processes that affect the biomass of phytoplankton and nutrients. They represent ecological processes through a set of complex nonlinear differential algebraic equations, with rate coefficients that require an estimation to suit site-specific environment. Therefore, the first step in the development of an eutrophication model is to solve a dynamic parameter estimation problem.

This problem has been addressed through different approaches. Zhang *et al*. (2004) have proposed a sequential procedure to determine phytoplankton and zooplankton parameters using exergy as the objective function and calibrating both physical and chemical parameters by trial and error. Shen and Kuo (1998) used the variational method for estimating unknown kinetic parameters. More recently, Shen (2006) proposed a least-squares objective function and the resolution of the dynamic parameter estimation problem through the application of a modified Gauss-Newton method.

In this work, we formulate a parameter estimation problem with a weighted least-squares objective function subject to a large-scale partial differential algebraic equations model resulting from temporal and spatial dynamic mass balances in the major groups of phytoplankton community (cyanobacteria, diatoms and chlorophyta), key nutrients in the eutrophication, biochemical demand of oxigen and dissolved oxygen. Algebraic equations represent profiles for temperature, solar radiation and river inflows, in addition to the calculation of most factors that affect rate equations, such as effect of solar radiation, temperature, nutrients, etc. The PDE is transformed into an ordinary differential equation system by spatially discretizing it into sets of ordinary differential-algebraic equations (DAE) (Rodriguez and Diaz, 2007). The DAE optimization problem is solved with a simultaneous approach.

The present study has been performed on Paso de las Piedras Reservoir, which supplies drinking water for two cities in Argentina. The discretized NLP problem has been solved with a reduced Successive Quadratic Programming algorithm (Biegler *et al.*, 2002). Numerical results show good agreement with values from the literature. The model is currently being validated with recently obtained additional data from the lake.

2. Study area and input data

Paso de las Piedras Reservoir is located in the south of Buenos Aires Province (Argentina) at 38° 22´ S and 61° 12´ W. It was built to supply drinking water to Bahía Blanca and Punta Alta (cities whose population is above 400,000 inhabitants) and for industrial purposes at a petrochemical complex nearby. The lake has two tributaries: El Divisorio and Sauce Grande River. The lake has a coastline perimeter of 60 kilometers and a mean depth of 8.2meter. Biological and chemical data have been weekly collected from January to December 2004 at four sampling stations. Biological qualitative and quantitative determinations have been carried out, as well as physicochemical ones, that

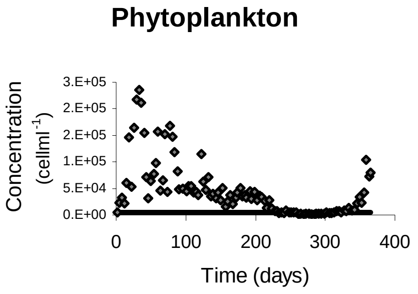

Figure 1. Measured phytoplankton concentr. and eutrophication limit (5000 cell/ml)

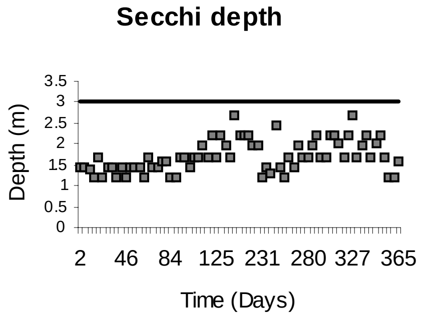

Figure 2. Measured Secchi disk depth (eutrophic state between 1 and 3 m)

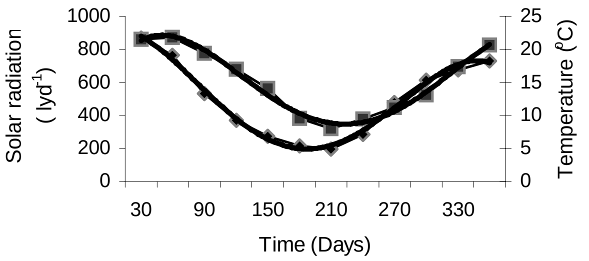

Figure 3. Temperature (°C) and solar radiation (lyd^{-1}) versus time.

include concentrations of nitrate, ammonium, organic nitrogen, phosphate, organic phosphorus, dissolved oxygen and biochemical demand of oxygen, water temperature, pH and depth of Secchi disk (depth at which the disk can be seen from outside the water body). The high content of phosphorus and nitrogen in Paso de las Piedras Reservoir is consequence of agricultural activities. The trophic level of this water body is currently eutrophic (Parodi *et al.*, 2004), as it can be clearly seen in Figs. 1 and 2. These figures show measured concentration profiles for phytoplankton and Secchi disk depth as related to the levels beyond which the water body is considered eutrophic (horizontal lines that correspond to 5000 cells/ml and 3 m, for phytoplankton concentration and Secchi disk depth)

Input requirements for the model are of four types. These are descriptive data for the lake itself, hydrodynamic forcing data (primarily meteorological, as temperature and solar radiation, and inflow and outflow profiles data), water quality known parameters, phytoplankton and nutrients profiles and initial conditions for all the modeled variables. High frequency sampling is required to properly describe the dynamics of the lake. The external forcing functions, such as temperature and solar radiation were approximated with polynomial functions (r^2=0.98 and 0.94, respectively), as shown in Fig. 3. River inflows and associated nutrient loading., as well as outflow data have also been approximated with polynomials.

3. Dynamic Parameter Estimation Problem

Eutrophication models comprise large sets of complex differential algebraic systems of equations (DAE). Therefore, the associated parameter estimation problem is formulated as a large-scale DAE-constrained optimization problem.

Partial differential equations arise from dynamic mass balances for each state variable. Main simplifying hypothesis are: constant transversal area in the lake, constant water density, phosphorus as limiting nutrient and horizontally averaged concentrations. In this way, only gradients along the water column height are considered. To transform partial differential equations system into an ordinary differential equations one, the column height is discretized into two layers, according to the available data. Data at different depths are currently being collected to develop a model with a higher number of water layers. In most eutrophication models, the different types of phytoplankton are lumped within one state variable, however, we have considered three state variables corresponding to diatoms, chlorophytes and cyanobacteria, because it is important to know the proportion in which they are present in an algal bloom, to determine the potential damage they can produce in the water drinking resource. The remaining state variables correspond to concentrations of main nutrients (nitrate, nitrite, ammonium, organic nitrogen, phosphate, organic phosphorus), dissolved oxygen and biochemical demand of oxygen.

Dynamic mass balances in each spatial layer include component inputs from tributaries, outputs for both potabilization and industrial purposes, generation and consumption, and transference between layers, also accounting for lake volume variability (through upper layer height variability). Estimated parameters are included within the generation/consumption terms. The three phytoplankton groups differ in their maximum growth rates, nitrogen and phosphorus kinetics and light requirements. Algebraic equations stand for profiles in temperature, solar radiation and river inflows. Additional equations have been written for the calculation of each component generation and consumption. The objective function is a weighted least squares one.

The resulting DAE constrained optimization problem is formulated within a simultaneous dynamic optimization approach, in which the DAE system is transformed into a large nonlinear programming (NLP) problem by representing state variables profiles by polynomial functions over finite elements in time. The NLP is then solved with an efficient reduced successive quadratic programming (rSQP) algorithm within program IPOPT (Biegler *et al.*, 2002).

Mass balances for horizontal layers
Upper layer

$$\frac{dC_{Uj}}{dt} = \sum_{k=1}^{NIN} \frac{QIN_{U,k}}{V_U} CIN_{Ujk} - \sum_{m=1}^{NOUT} \frac{QOUT_U}{V_U} C_{Uj} + r_{Uj} - \frac{kdA}{\Delta h_U h_U}(C_{Uj} - C_{Lj}) - \frac{C_{Uj}}{h_U}\frac{dh_U}{dt}$$

Lower layer

$$\frac{dC_{Lj}}{dt} = \sum_{m=1}^{NOUT} \frac{QOUT_L}{V_L} C_{Lj} + r_{Lj} + \frac{kdA}{\Delta h_L h_L}(C_{Lj} - C_{U,j}) - \frac{C_{Lj}}{h_L}\frac{dh_L}{dt} \text{ Lower layer}$$

Rate equations for phytoplankton (*rij*; *i*=upper, lower layer: *j*= cyanobacteria, diatoms, cyanophytas)

$$r_{ij} = R_{ij,growth} - R_{ij,resp} - R_{ij,death} - R_{ij,sedim}$$

$$R_{ij,growth} = k_{j,growth} * f(T) * f(I) * f(N) * C_{ij}$$

$$f(T) = \frac{Temp}{Tempj} exp(1 - \frac{Temp}{Tempj}) \quad f(I) = \frac{I}{Ij} exp(1 - \frac{Ii}{Ij}) \quad f(N) = \frac{C_{iPO4}}{C_{iPO4} + kpj}$$

$$R_{ij,resp} = k_{j,resp} * C_{ij} \quad R_{ij,death} = k_{j,death} * C_{ij} \quad R_{ij,sedim} = k_{j,sedim} * \frac{1}{h_i} * C_{ij}$$

Rate equations for phosphate (*rij*; *i*=upper, lower layer: *j*=phosphate)

$$r_{ij} = R_{ij,death} + R_{ij,miner} - R_{ij,uptake}$$

$$R_{ij,death} = \sum_{m=1}^{3} (a_{pc} * k_{m,death} * (1 - f_{po}) * C_{im})$$

$$R_{ij,miner} = k_{miner} * \theta_{miner} * exp(Temp - 20) * \frac{\sum_{m=1}^{3} C_{im} * C_{iOP}}{km_{pc} + \sum_{j=1}^{3} C_{im}}$$

$$R_{ij,uptake} = \sum_{m=1}^{3} (R_{im,growth} * a_{pc} * C_{im})$$

Rate equations for nitrate (r_{ij}; *i*=upper, lower layer: *j*=nitrate)

$$r_{ij} = R_{ij,nitri} - R_{ij,uptake} - R_{ij,denitr}$$

$$R_{ij,nitri} = k_{nitri} * \theta_{nitri} * exp(Temp - 20) * \frac{C_{iNH4} * C_{iDO}}{k_{nio} + C_{iDO}}$$

$$R_{ij,denitr} = k_{denitr} * \theta_{denitr} * exp(Temp - 20) \frac{C_{iNO_3} * k_{no3}}{k_{no3} + C_{iDO}}$$

$$R_{ij,uptake} = \sum_{m=1}^{3} (a_{nc} * R_{im,growth} * (1 - PNH4) * C_{im}))$$

Additional rate equations have been written for the remaining components. Parameters of the model are of three types: kinetic, stoichiometric and physical.

4. Discussion of Results

The resulting parameter estimation problem to determine the values of nine parameters in the Paso de las Piedras eutrophication model has twenty differential equations and fifty algebraic ones, after spatial discretization in two layers. Currently available weekly measurements of concentrations at two water levels (water surface and outflow level, at six meters depth) have rendered this discretization. A time horizon of 365 days has been considered to account for a complete annual cycle. The resulting nonlinear programming (NLP) problem for forty elements and three collocation points has 10432 nonlinear equations. It has been solved with an Interior Point method with reduced Successive Quadratic Programming (rSQP) techniques within program IPOPT (Biegler *et al*., 2002; Raghunathan *et al*., 2004), in which successive parametric NLP subproblems are solved for decreasing values of the barrier parameter. Initial barrier parameter value has been 0.01. Estimated parameters are shown in Table 3. Their values give state variables profiles which are in agreement with data from the lake. Figure 3 shows cyanobacteria, diatoms, nitrate and phosphate profiles as compared to experimental data for an entire cycle of 365 days.

Table 3. Optimal parameter set for eutrophication model

Symbol	Description	Calibrated value
$k_{C,growth}$	Max growth of cyanobacteria (d^{-1})	0.210
I_C	Optimal growth radiation of cyano (lyd^{-1})	109.9
$k_{D,growth}$	Max growth of diatoms (d^{-1})	0.405
I_D	Optimal growth radiation of diatoms (lyd^{-1})	24.52
$K_{G,growth}$	Max growth of chlorophytes (d^{-1})	0.654
I_G	Optimal growth radiation chlorophytes (lyd^{-1})	89.74
$k_{ON,miner}$	Rate coeff. mineralization ON(d^{-1})	0.0922
$k_{OP,miner}$	Rate coeff. mineralization OP(d^{-1})	0.0149
k_{nio}	Half-sat. conc. for oxygen lim. of nitrification (mgl^{-1})	0.3430

5. Conclusions

The parameter estimation problem for an eutrophication model has been solved with a simultaneous dynamic approach. To our knowledge, these rigorous models have not been solved with advanced dynamic optimization techniques. A large number of biological parameters has been determined, based on weekly measurements throughout 2004. No data reconciliation has been required at this stage. Currently, more detailed data are being obtained at different water levels to formulate a more detailed model.

Once validated, the dynamic optimization model will be run to determine optimal profiles for nutrient inputs to establish remediation policies.

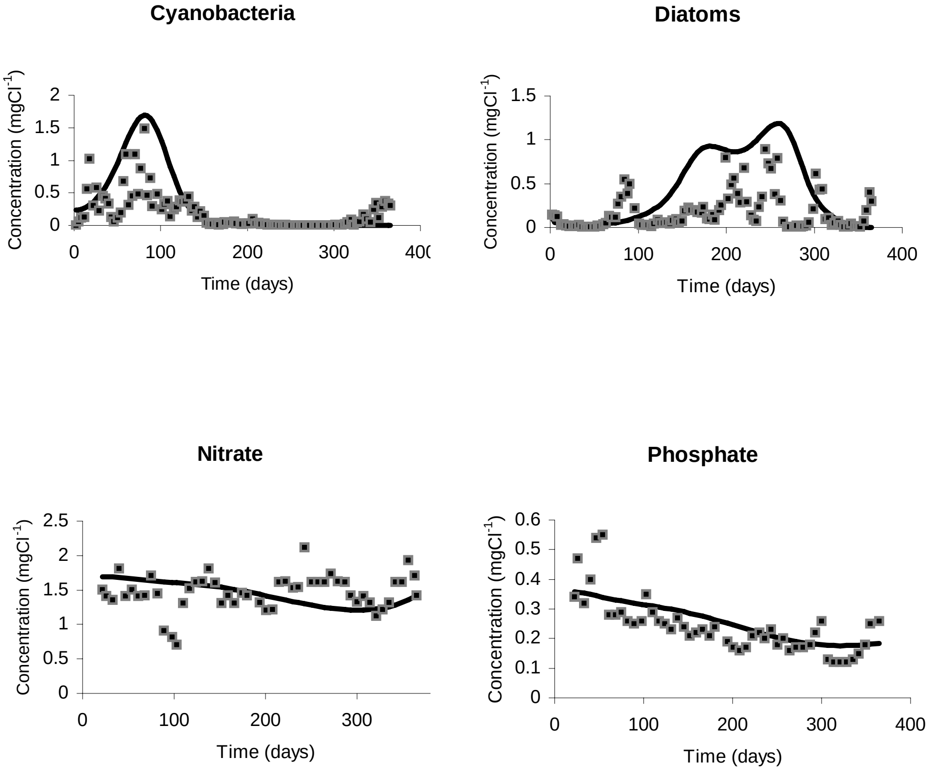

Figure 3. Experimental data and simulated profiles (continuous line) with estimated parameters

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