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Dynamic Parameter Estimation Problem For A Water Quality Model

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This work deals with the parameter estimation problem for a lake eutrophication model. The model is a dynamic parameter estimation one, which is solved with a simultaneous approach with an nonlinear programming solver. Gradients of state variables are considered in the vertical direction, rendering a partial differential equation problem which is transformed into a differential algebraic (DAE) one by spatial discretization in two water layers. Main biochemical and chemical parameters have been obtained, which allow a close representation of the lake dynamics.

1. Introduction

The need for predictive ecological water quality modeling has arisen as a result of the increasing eutrophication of lakes throughout the world. 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 calibration to suit site-specific conditions. Consequently, the first step in an eutrophication model development is the resolution of a parameter estimation problem.

The parameter estimation problem in eutrophication models 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 capable of handling upper and lower bounds on parameters and the Hessian being approximated with information from the sensitivity matrix calculated by finite differences.

In this work, we formulate a parameter estimation problem with a least-squares objective function subject to a large-scale partial differential algebraic equations (PDE) model resulting from temporal and spatial dynamic mass balances in phytoplankton in the form of diatoms, green algae and cyanobacteria; dissolved oxygen and nutrients, such as nitrate, ammonium, organic nitrogen, silica, phosphate and organic phosphorus. 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, nutrients, etc. The PDE is transformed into an ordinary differential equation system by spatially discretizing the PDE into sets of ordinary differential-algebraic equations (DAE) (Rodriguez and Diaz, 2006). The DAE optimization problem is then transformed into a large nonlinear programming (NLP) problem by representing state and control variables profiles by polynomial functions over finite elements in time. Data sets from an entire year have been included.

The present study has been performed on Lake Paso de las Piedras, a lake that supplies drinking water for more than 400,000 inhabitants. The high content of phosphorus and nitrogen in Paso de las Piedras Lake is consequence of agricultural activities. 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. Lake description

Lake Paso de las Piedras (Fig. 1) is located in the south of the Buenos Aires Province (Argentina) at 38° 22´ S and 61° 12´ W and was constructed to supply drinking water to the cities of Bahía Blanca and Punta Alta and for industrial purposes at a petrochemical complex nearby.

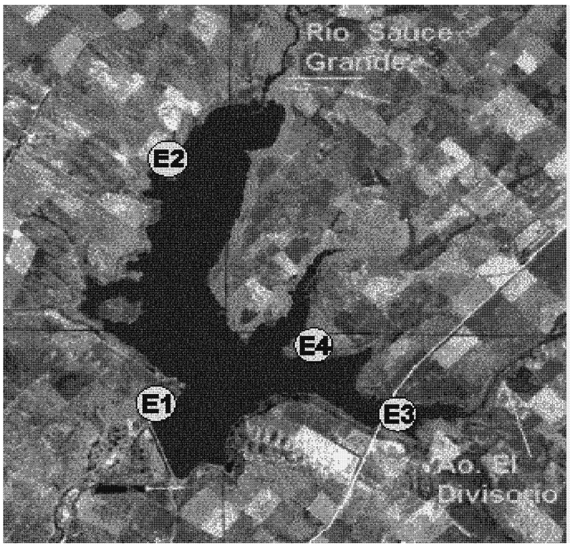

Figure 1. Satellite image of Lake Paso de las Piedras indicating the tributaries and the sampling sites (E_1, E_2, E_3 and E_4).

The trophic level of this water body currently corresponds to eutrophic category and it undergoes algal blooms during warm months. The Stream El Divisorio and Sauce

Grande River are the two tributaries of the lake. A summary of lake characteristics is shown in Table 1. Biological and chemical data were weekly collected from January to December 2004 at four sampling stations (Fig 1).

Table 1. Lake characteristics

Area of drainage basin	1620 km2	Maximum depth	28 m
Perimeter of coastline	60 km	Maximum volume	328 Hm3
Surface	36 km2	Retention time	4 years
Mean depth	8.2 m		

3. Parameter Estimation Problem for Eutrophication and Data Input

Mechanistic eutrophication models represent ecological processes by partial differential inter- dependent conservation equations, with rate coefficients that require calibration to suit site-specific conditions. Therefore, the first step in an eutrophication model development is the formulation and solution of a dynamic parameter estimation problem.

In this work, we have formulated a one dimensional dynamic model for the lake, which has been spatially discretized in two layers, corresponding to currently available concentrations data at two levels in the lake.

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 2. River inflows and associated nutrient loading., as well as outflow data have also been approximated with polynomials. Future improvements include their representation with sinusoidal functions.

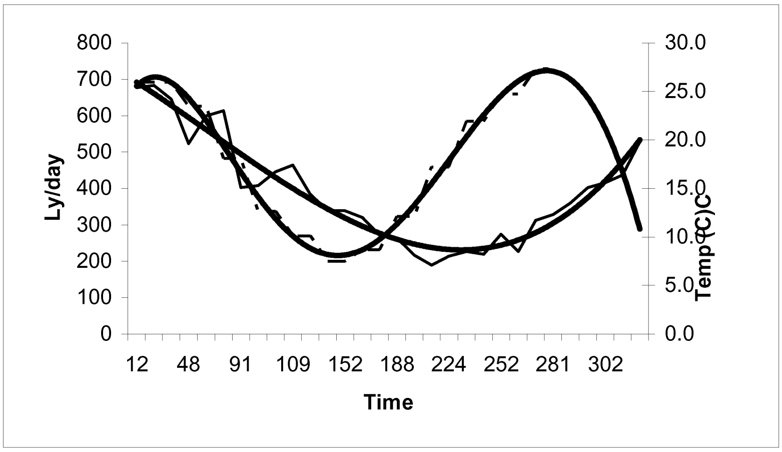

Figure 2. Temperature and solar radiation versus time.

Additional inputs for the parameter estimation problem includes concentration profiles for the modeled state variables, i.e., three groups of phytoplankton, nitrogen as nitrate, ammonium and dissolved organic nitrogen, phosphorus, as orthophosphate and dissolved organic phosphorus, oxygen as dissolved oxygen and biochemical oxygen demand. Weekly data throughout a whole year have been included.

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 how they are present in a bloom of algae, in order to determine the potential damage that they can produce in the water drinking resource.

Differential equations for each state variable in each spatial layer include components inputs from tributaries, outputs for both potabilization and industrial purposes, sources and sinks, transference between layers, as well as accounting for lake volume variability. Estimated parameters are included within the source and sink terms. They are listed in Table 3, together with their estimated values. The three phytoplankton groups differ in their maximum growth rates, nitrogen and phosphorus kinetics, light requirements.

$$\frac{dCi,j}{dt} = \frac{(QUCi\ in - QUoutCi)}{Vj} + Si,j - \frac{kd * A}{\Delta DU * VU}(Ci,U - CiL) - \frac{CiU}{DU}\frac{dDU}{dt}$$

$$Si,j = (\mu i,j - ri,j - mi,j - vsi / Dj)Ci$$

$$\begin{aligned} \mu i,j &= \mu maxi * fTi,j * fNi,j * fIi,j \\ fTi,j &= (temp/tempi) * exp(1 - (temp/tempi)) \\ fNi,j &= (PO4j/(PO4j + kpi)) \\ fIi,j &= (Lj/Li) * exp(1 - (Lj/Li)) \end{aligned}$$

where,

Ci, j = concentrations of i (g/m^3)

QU and $QUout$ = input and output rate (m3/d)

Si, j = rate of change of i (Zhang *et al*. 2004, Zheng *et al.* 2004) (g/m^3/d)

i = diatoms, chlorofites, cyanobacteria, NO_3, NH_4, NO, PO_4, PO, DO and DBO

j = different layers at the water column

DU and VU= depth (m) and volume (m^3) of upper layer respectively

A = surface area (m^2)

kd = mixing rate (m^2/d)

$\mu i,j$ = net growth (1/d)

fT, fN and fI = effects of water temperature, nutrients and solar radiation, respectively

$\mu imax$ = maximum growth of i (1/d)

ri = respiration rate of i

mi = mortality rate of i (1/d)

vsi = settling velocity of i (1/d)

tempi = optimum temperature of growth of *i* (C)
Li = optimum solar radiation of growth of *i*(Ly/d)
kpi = half saturation constant for phosphorus uptake (g/m^3)

4. Discussion of Results

The parameter estimation problem to determine the values of twelve parameters in the Paso de las Piedras eutrophication model is a differential algebraic optimization model with twenty differential equations and fifty algebraic ones, after spatial discretization in two layers. The objective function is a least squares one. Currently available weekly measurements of concentrations at two water levels (water surface and outflow level, at eight meters depth) have rendered this discretization. At the moment, data are being collected at six different levels to perform a more detailed 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 (SQP) techniques within program IPOPT (Biegler et al., 2002), 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, which are within upper and lower bounds from the bibliography, give state variables profiles which are in agreement with data from the lake. Figure 3 shows cyanobacteria and nitrates profiles as compared to experimental data for an entire cycle of 365 days.

Table 3

Symbol	Description	Calibrated value	Lower bound	Upper bound
μ_{Cmax}	Max growth of cyanobacteria (l/d)	4.502	1.30	4.50
m_C	Mortality rate of cyanobacteria (1/d)	0.041	0.001	0.125
$temp_C$	Optimal growth temp. of cyano (C)	27.010	15	30
μ_{Dmax}	Max growth of diatoms (l/d)	3.011	1.30	4.50
m_C	Mortality rate of diatoms (l/d)	0.101	0.001	0.125
$temp_D$	Optimal growth temp. of diatoms (C)	15.212	15	30
μ_{Gmax}	Max growth of chlorophytes (l/d)	2.903	1.30	4.50
m_C	Mortality rate of chlorophytes (l/d)	0.098	0.001	0.125
$temp_G$	Optimal growth temp.chlorophytes(C)	23.564	15	30
kni	Rate coeff. for nitrification (1/d)	0.0035	0.005	0.030
kmP	Rate coeff. mineralization OP(1/d)	0.040	0.002	0.400
vsNO	Settling rate of ON (1/d)	0.051	0.002	0.090

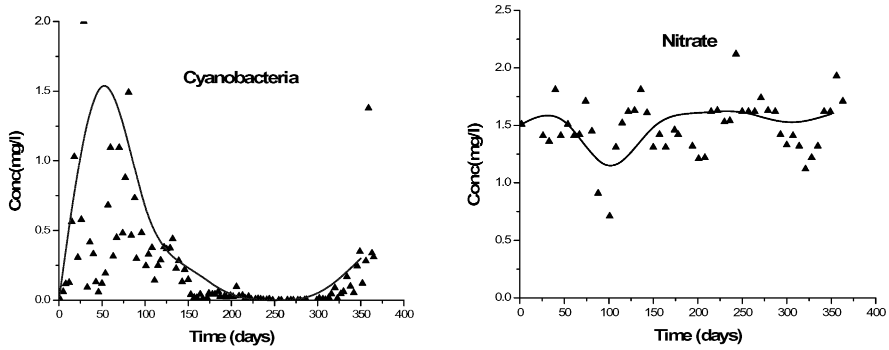

Figure 3. Experimental data (▲) and simulated profiles (continuous line) with estimated parameters

5. Conclusions

A dynamic 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. 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.

Acknowledgments

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