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Biological Wastewater Treatment: Dynamic Global Sensitivity Analysis and Parameter Estimation in a System of Waste Stabilization Ponds

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Abstract

In this work, we propose a dynamic mathematical model describing main biochemical processes that take place within wastewater stabilization ponds. Mass balances for main microorganisms, nutrients, dissolved oxygen and biochemical demand of oxygen have been formulated. The wastewater biological treatment system under study is composed of two stages of oxygenated ponds in series. The first stage is aerobic oxygenated and the last one is facultative oxygenated. Global sensitivity analysis has been performed prior to the formulation of a parameter estimation problem, subject to the differential algebraic system describing the biological wastewater treatment system. Experimental data from a fruit juice plant have been collected throughout one year. Numerical results provide a deep insight on the complex relations among microorganisms, nutrients and organic matter concentration in wastewater treatment ponds.

Keywords: biological wastewater treatment, parameter estimation

1. Introduction

The sustainable provision of fresh water is one of the main challenges in this century. In this sense, wastewater treatment processes constitute a main issue to minimize major adverse impacts on freshwater and coastal ecosystems asssociated to urban and industrial growth. Activated sludge processes are currently the most widely used biological processes. Stabilization ponds, in turn, are large lagoons where wastewater is stored for long periods to allow a wide range of microorganisms to break down organic matter and sludge is not returned. Waste stabilization ponds can be a combination of three different pond types: anaerobic, facultative and maturation. Facultative ponds can be classified into primary (inflows without treatment) and secondary (inflows with pre-treated in anaerobic ponds). In these ponds, there are aerobic, facultative and anaerobic zones, and different chemical and biochemical processes take place within the different zones, including mutualistic relationships between microalgae, heterotrophic bacteria and fungi that greatly influence the pond efficiency in biological wastewater treatment. A few models have been proposed for waste stabilization ponds describing hydrodynamic (Manga et al., 2004, Shilton and Mara, 2005) or biochemical processes (Kayombo et al., 2000; Dochain et al., 2003). However, the different pollutant removal processes have yet not been entirely understood.

In this work, we address the formulation of a detailed mechanistic model for a system of stabilization ponds (aerobic and facultative) for control purposes. Dynamic mass balances are formulated for bacteria, yeast, main groups of phytoplankton, nitrogen, phosphorus, dissolved oxygen and biochemical demand of oxygen. Global sensitivity analysis has been performed applying Sobol´ method (Sobol, 2001) to determine most influential parameters. Based on these results, a parameter estimation problem has been formulated, subject to the differential algebraic system describing the biological wastewater treatment system. Collected data from a juice plant have been used for parameter estimation (frequency of fifteen days in the intensive working period). Numerical results provide useful information on the complex relations among microorganisms, nutrients and organic matter concentration.

2. Biological treatment system model

In wastewater stabilization ponds, microrganisms are used under controlled conditions to rapidly oxidize organic matter in wastewater to innocuous end products that can be safely discharged to surface water. The wastewater biological treatment system under study is composed of three stages of oxygenated ponds in series within a juice plant in Argentina. The first two ponds are aerobic oxygenated and the last one is facultative oxygenated. Figure 1 shows their spatial distribution.

Figure 1. System of wastewater stabilization ponds

The facultative pond has been modeled as composed of two horizontal layers, to represent dissolved oxygen concentration gradient along the water column, as well as the different associated processes taking place in each zone (Estrada et al., 2009). A global mass balance is formulated for each pond, taking into account the wastewater stream and rain as inflows and the treated stream and evaporation as outflows. Dynamic mass balances are formulated for bacteria, yeast, main groups of phytoplankton (cyanobacteria, diatomea, chlorophyta), nitrogen as nitrate, ammonium and organic nitrogen, phosphorus as phosphate and organic phosphorus, dissolved oxygen and biochemical demand of oxygen, as follows:

$$\frac{dC_{ij}}{dt} = \frac{Q_{in_i}}{V_i} C_{in_{ij}} - \frac{Q_{out_i}}{V_i} C_{ij} + r_{ij} - \frac{k_d A_i}{\Delta h\, V_i} \left(C_{Uj} - C_{Lj}\right) - \frac{C_{ij}}{h_i} \frac{dh_i}{dt} \quad (1)$$

i=L, U (horizontal layer in facultative pond)

j= bacteria, yeast, cyanobacteria, diatomea, chlorophyta, nitrate, ammonium, organic nitrogen, phosphate, organic phosphorus, dissolved oxygen, biochemical demand of oxygen

Bacteria play a fundamental role in biological wasterwater treatment as they are primarily responsible for the oxidation of organic matter. Equations that describe bacteria dynamics are as follows (Beran y Kargi, 2004):

$$r_{ij} = R_{ij,growth} - R_{ij,metabolism} - R_{ij,settling} - R_{ij,predation}, j{=}B \quad (2)$$

For bacteria (B), the growth term is dependent on biochemical demand of oxygen (BDO), dissolved oxygen concentration (DO), pH, temperature, limiting nutrien concentration (N) and bacteria concentration, as:

$$R_{ij,growth} = u_{max,j} * f(BOD)_{ij} * f(DO)_{ij} * f(pH)_{ij} * f(T)_{ij} * f(N)_{ij} * C_{ij},\ j{=}B \quad (3)$$

Dependence on *BOD*, *DO* and *pH* are of Monod type.

$$R_{ij,metabolism} = bm_j * \theta_{m,j}^{(T-20)} * C_{ij} \qquad j{=}B \quad (4)$$

$$R_{ij,settling} = vs_j * \frac{1}{h_i} * C_{ij} \qquad j{=}B \quad (5)$$

$$R_{ij,predation} = pr_j * C_{ij} \qquad j{=}B \quad (6)$$

where u_{maxB} stands for the maximum growth rate for bacteria and bm_B, vs_B and pr_B are parameters associated to bacteria basal metabolism, settling and predation, while θ_{mB} is the temperature dependence factor for bacteria.
Phytoplankton provide oxygen for bacterial breakdown of organic matter. Consumption and generation terms (r_{ij}) describing phtoplankton dynamics are presented in Estrada et al. (2009), considering a growth term where the maximum growth rate is affected by limitation functions in a multiplicative model including nutrient concentration, light intensity, temperature and pH (this factor has been included in previous work). Yeast enter the ponds with the wastewater treatment stream, as this stream comes from washing the processed fruit (mainly pears and apples). Finally, it is important to note that wastewater can be treated biologically only if certain ratios among carbon, nitrogen and phosphorus are obtained. If that is not the case, the addition of certain nutrients becomes necessary. Equations for BDO, DO and nutrient concentrations can be found in Estrada et al. (2009). Algebraic equations in the model represent rate equations and profiles for temperature, solar radiation, pH, inflows, concentrations, etc. The model representing the aerobic and facultative ponds has thirty three differential equations and eighty six algebraic ones.

3. Global Sensitivity Analysis and Parameter Estimation

As a first step, we have perfomed global sensitivity analysis on the differential algebraic system (DAE) representing the system of wastewater stabilization ponds. First order sensititvity indices of variable y with respect to parameter x_i (S_i) have been estimated as:

$$S_i = \frac{V(E(y|x_i))}{V(y)} = \frac{V_i}{V(y)} \quad (7)$$

with the methodology proposed by Sobol at each time point (Sobol, 2001, Saltelli and Tarantola, 2002, Estrada & Diaz, 2010). Stochastic simulations have been carried out in gPROMS (PSEnterprise) and matrices with results for the different scenarios have been exported for indices calculation in a Fortran 90 environment. We have studied parameter sensitivity on main state differential variables related to stabilization ponds; they are biochemical demand of oxygen (BDO, representing organic matter content), bacteria concentration and dissolved oxygen concentration (DO, associated to required power from aerators). Parameter sensitivity on nutrient and phytoplankton has been studied in previous work (Estrada & Diaz, 2010).

Global sensitivity results have provided a set of main parameters to be determined based on collected data from a juice plant along one year. The objective function is a maximum likelihood one subject to the DAE system that stands for the model representing the system of stabilization ponds.

4. Discussion of results

Global sensistivity analysis has been carried out, considering a thousand scenarios to provide a set of identifiable parameters in the stabilization ponds system. Table 1 shows main parameters affecting bacteria concentration and biochemical demand of oxygen concentration in at two time instants: day=50, within the phase of low production and day=200, within a high production period. We have also analyzed sensitivity indices for dissolved oxygen concentration, phytoplankton and nitrate and ammoniumm concentration. It can be noted that the set of main parameters has 20 parameters; it includes u_{maxB}, $u_{maxCyano}$, y_{ocB} (oxygen to biomass ratio in bacteria), bm_B, θ_{mB} (all shown in Table 1), as well as parameters involved in rate equations for dissolved oxygen, phytoplankton and nutrients.

Table 1. First order sensitivity indices for bacteria and BDO concentration at 50 days (low production period) and at 200 days (high production period)

Bacteria concentration			BDO (biochemical demand of oxygen)		
Parameter	t=50 days	t=200 days	Parameter	t=50 days	t=200 days
u_{maxB}	0.011	0.355	u_{maxB}	0.021	0.123
bm_B	0.003	0.092	y_{ocB}	0.134	0.213
$u_{maxCyano}$	0.087	0.098	θ_{mB}	0.153	0.247

Concentration data for the eleven components have been collected from the aerobic and facultative (upper and lower layer) ponds along one year, starting in August 2010 (time=0), with higher frequency during the summer (days 150 to 250), which is the period of intensive production. The parameter estimation problem has been formulated within a sequential approach (gPROMS, PSEnterprise, 2010) to estimate the twenty parameters determined as most influential in the global sensitivity analysis. Part of them are shown in Table 2. The problem converged in seventy iterations, with weighted residual slightly lower than chi-squared value.

Table 2. Main estimated parameters in system of stabilization ponds

Parameter	Initial value	Opt. value	Parameter	Initial value	Opt. value
$u_{max,B}$	0.65	0.85001	K_{nitrif}	3.00	3.49361
bm_B	0.03	0.04498	$\theta_{m,nitrif}$	1.08	1.12488
$u_{max,Cyano}$	0.23	0.29722	$\theta_{m,B}$	1.11	1.15113

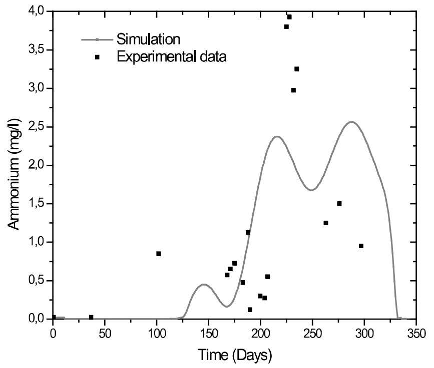

Figure 2. Ammonium concentration profile.

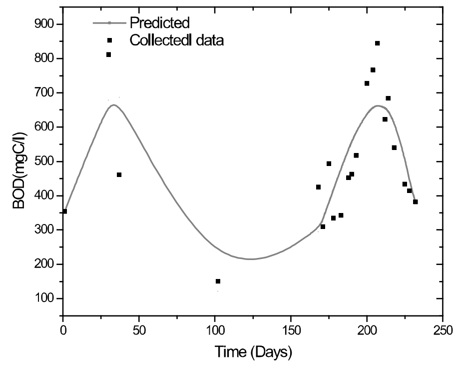

Figure 3. BOD concentration profiles: Collected data and simulation values.

Figures 2 and 3 show good agreement between estimated concentrations for ammonium and biochemical demand of oxygen and collected data.

5. Conclusions

We have addressed the formulation of a mathematical model for a system of biological wastewater treatment ponds with the inclusion of dynamic mass balances for the main microorganisms involved in biochemical processes taking place within stabilization ponds; ie., bacteria, phytoplankton and yeast. Well-known processes as nitrification and denitrification are also modeled. A global sensitivity analysis has determined main parameters that have been estimated based on collected data from a system of stabilization ponds in a fruit juice plant. The formulation of an optimal control problem for energy consumption minimization is part of current work.

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