MODELING AND DETECTION OF STRUCTURAL CHANGE IN THE DYNAMICS OF DO IN A SOUTHEASTERN PIEDMONT IMPOUNDMENT

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Abstract. A modified Recursive Prediction Error (RPE) algorithm is used to discover structural change in modeling dynamics of dissolved oxygen (DO) in an aquaculture pond. The small aquaculture pond with a surface area of 1.75 acres, located at Whitehall Forest near the University of Georgia campus, was fertilized on three occasions during the summer of 2000. System responses to nutrient addition have been observed using the University of Georgia's Environmental Process Control Laboratory (EPCL) for a continuous five-month period with 15-minute sampling intervals. A subset of these data – for a period of 36 days from July 1st through August 5th, 2000 – is examined in detail to observe and understand the dynamics of photosynthesis and DO *in situ*. A mechanistic model performs quite well for describing the concentrations of algae and DO during an algal bloom condition but poorly after the bloom ends. The results of recursive estimation indicate that another process, probably photosynthesis and respiration of macrophytes, may dominate the diurnal variation of DO when the algal biomass in the water column becomes negligible.

INTRODUCTION

An environmental system is always subject to changes regardless of an observer's awareness. A model, an approximation of the *true* system, is not able to track the evolutionary trajectory of the system due to its *fixed* structure when (apparent) structural changes emerge to be of significance. A *fixed* model structure is expressed by various state variables symbolizing the state of the *true* system and by the parameters connecting those state variables. Any changes in the *true* system brought about by the emergence or disappearance of a state variable or any progression of the connections (parameters) between these states can cause a model to fail. So we need a method of solution that can test the "success" or "failure" of any of the individual, constituent hypotheses - the ways in which the states are connected to each other - that are included in the model. Recursive state-parameter estimation algorithms can be used for this purpose (Beck, 1987). Among all these state-parameter estimation methods, the Recursive Prediction Error (RPE) filter is designed solely for parameter estimation and model structure identification (Beck *et al.*, 2002, Stigter, 1997). After being modified in Lin (2003) the RPE can be easily extended to *time-varying* parameter estimation cases.

A pond experiment was conducted in the summer of 2000. Up to 12 water quality variables (Lin, 2003; Parker *et al.*, 2003) were continuously monitored with the assistance of the EPCL and supporting equipment in sub-hourly sampling intervals. The system was limed on July 2nd and fertilized on July 5th, July 27th and October 1st. A subset of these data is examined for modeling and detection of structural change in the dynamics of DO in the pond.

MODEL PRESENTATION

In order to achieve model structure identification and parameter estimation with a reasonable chance of success, the model must be very simple, with a few parameters. Three main hypotheses are made. Firstly, it is assumed that the pond water is completely mixed. This assumption was verified by the fact that the temperatures taken at 0.5 m, 1m and 2m below water surface are almost the same from late June to the end of recordings. During the pond experiment the sampling pumps of the EPCL may act as a stirring force for circulating the pond water. Secondly, nutrients are supposed not to be rate limiting. During the observed time period (from July 1st to August 5th, 2000), two fertilizations were applied to the pond (Lin, 2003; Parker, 2003). The concentration of inorganic nitrogen in the water column is well above the half-saturation constant of 15 $\mu g \cdot L^{-1}$ (Thomann and Mueller, 1986) and the concentrations of orthophosphate also greatly exceed the half-saturation constant of 2.5 $\mu g \cdot L^{-1}$ (Thomann and Mueller, 1986). We therefore only consider light energy and temperature as growth controlling factors. Thirdly, the pond volume is assumed to be constant throughout the period during which the model is applied. This assumption is moderately reasonable. During the considered time period, only a one-inch rainfall occurred in the afternoon of July 23rd, 2000, and a 1.5 inches rainfall in the afternoon of July 30th, 2000. The water level of the Whitehall pond almost never reached the outlet during the entire experiment and the loss of water by evaporation could be compensated through the small influent flow originating from springs along the sides of the channel (Lin, 2003).

In a pond, the DO evolution depends on the balance between photosynthetic production, total consumption, and exchanges with the atmosphere. The gain and loss due to respective algal photosynthesis and respiration are calculated based on the Redfield stoichiometric coefficients. The DO consumed by the degradation of other organic matter in the water column is simply represented by that participating in the decomposition of the biodegradable organic carbon (measured as a portion of Total Organic Carbon (TOC)). While respiration and nonpredatory mortality of phytoplankton are often described as first-order reactions, zooplankton grazing and settling of phytoplankton are much more complicated processes. A *time-varying* parameter is employed to track the composite variation of these complicated processes responsible for the losses of algal biomass, including zooplankton grazing and settling to sediments. Similarly, other sources of the dissolved oxygen (e.g., from photosynthesis of macrophytes) are represented by another *time-varying* parameter. Table 1 gives details of the state variables, parameters and the environmental functions associated with the mechanistic model elucidating the dynamics of algae and dissolved oxygen in the Whitehall pond in details.

Table 1. Model formulations, variables and parameters

Formulations:

$$\frac{dx_1(t)}{dt} = k_1 f(I;t) f_1(T;t) x_1(t) - k_2 f_2(T;t) x_1(t) - k_3(t) \quad (1)$$

$$\frac{dx_2(t)}{dt} = ck_1 f(I;t) f_1(T;t) x_1(t) - ck_2 f_2(T;t) x_1(t) + k_6 f_3(T;t)(C_S(T;t) - x_2(t)) - k_4 f_4(T;t) C_{TOC}(t) + k_5(t) \quad (2)$$

$$f(I;t) = \frac{I(t)}{I_S} \exp\left(1 - \frac{I(t)}{I_S}\right) \text{(Steele, 1974)} \quad (3)$$

$$f_i(T;t) = q_i^{T(t)-20};\ i = 1, 2, 3, 4 \quad (4)$$

$$C_S(T;t) = 14.589 - 0.40T(t) + 0.008T(t)^2 - 0.0000661T(t)^3 \text{ (Mortimer, 1981)} \quad (5)$$

State variables and initial values:			
$x_1(t)$	Algal biomass concentration	4.41	$mg \cdot L^{-1}$
$x_2(t)$	Dissolved oxygen concentration	7.04	$mg \cdot L^{-1}$
Environmental (forcing) variables:			
$I(t)$	Solar radiation (light intensity) at 0.5 m below surface		$KJ \cdot m^{-2} \cdot h^{-1}$
$T(t)$	Water temperature		°C
$C_{TOC}(t)$	Total organic carbon concentration		$mg \cdot L^{-1}$
Fixed parameters:			
c	Redfield stoichiometric coefficient	3.47	—
I_S	Saturation solar radiation	80	$KJ \cdot m^{-2} \cdot h^{-1}$
k_6	Global transfer coefficient between air and water at 20°C	0.4	d^{-1}
q_1, q_2, q_3, q_4	Correction factors for temperature	1.025, 1.02, 1.02, 1.02	
Time-invariant parameters and initial values:			
k_1	Specific growth rate of algae at 20°C	2.4	d^{-1}
k_2	Kinetic rate of loss of algae due to respiration and nonpredatory death	0.48	d^{-1}
k_4	Total organic matter decay rate	0.6	d^{-1}
Time-varying parameters and initial values:			
$k_3(t)$	Loss of algae due to grazing and settling processes, etc.	0	$mg \cdot L^{-1} \cdot d^{-1}$
$k_5(t)$	Sources of DO other than re-aeration and *algal* photosynthesis	0	$mg \cdot L^{-1} \cdot d^{-1}$

RECURSIVE PARAMETER ESTIMATION AND DETECTION OF STRUCTURAL CHANGE

In order to apply the RPE algorithm to the model for the dynamics of algae and DO in the Whitehall pond, the model with formulations (1)-(5) (see Table 1) is rewritten in the innovations representation (6a) with a linear observation equation (6b) since both algal biomass (through chlorophyll-*a*) and DO concentrations are observed directly.

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{\text{á}}; t) + \mathbf{K}\mathbf{\text{í}}(t) \quad (6a)$$

$$\mathbf{y}(t_k) = \mathbf{H}(\mathbf{\text{á}}; t_k)\mathbf{x}(t_k) + \mathbf{\text{í}}(t_k) \quad (6b)$$

where, $\dot{\mathbf{x}}(t) = [dx_1(t)/dt, dx_2(t)/dt]^T$; $\mathbf{u}(t) = [I(t)]$, the input function to the pond system; $\mathbf{x}(t) = [x_1(t), x_2(t)]^T$; $\mathbf{y}(t_k) = [y_1(t_k), y_2(t_k)]^T$, the observations of algal biomass and DO concentrations, respectively; $\mathbf{\text{á}}(t) = [k_1, k_2, k_3(t), k_4, k_5(t)]^T$; $\mathbf{\text{í}}(t_k) = [n_1(t_k), n_2(t_k)]^T$, the measurement noises and disturbances reflected in the observations of algal biomass and DO; $\mathbf{K} = \begin{bmatrix} K_{1,1} & K_{1,2} \\ K_{2,1} & K_{2,2} \end{bmatrix}$, Kalman-like gain matrix, which distributes the impacts of mismatches among the constituent representations of the state variable dynamics; $\mathbf{H}(\mathbf{\text{á}}; t_k) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, observations matrix, and the two entities of vector $\mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{\text{á}}; t)$ are Equations (1) and (2) respectively in Table 1.

Shown in Table 1, parameters k_1, k_2, k_4 are assumed to be time invariant over the period studied, while the values of $k_3(t)$ and $k_5(t)$ are allowed to change with time. The variations of these *time-varying* parameters are modeled by *Random Walk* (RW) stochastic processes since no *a priori* knowledge is available. Whether the recursive estimates of the time-invariant parameters' evolution change with time reveals the adequacy or inadequacy of the associated individual constituent hypotheses. The trajectories of the *time-varying* parameters also provide clues for constructing new hypotheses. The four elements in **K** are considered as time-invariant parameters as well. Their values are set to be zeroes initially implying that the mechanistic model describes the dynamics of algae and DO perfectly. Any excursions of the recursive estimation of **K**'s elements from zero suggest *apparent* structural change (Beck *et al.*, 2002).

RESULTS AND DISCUSSION

Having specified the initial conditions for all states and parameters, initial covariance matrices for all parameters and the variance matrix for measurement errors (Lin, 2003), the modified RPE algorithm has been applied to the simple model (1)-(5) of the dynamics of algal biomass and DO in the pond. Figure 1 displays the one-step-ahead predictions of the model against the observations of algal biomass and DO concentration. The model tracks the behavior of algae remarkably well (Figure 1a) the peak and the diel characteristics of the algal growth are caught by the model, although the model results are those of the one-step-ahead predictions. However, the discrepancy between the model and the observations of DO is not insignificant (Figure 1b). The model captures the diurnal oscillation pattern quite precisely but misses the alteration of amplitude. A few matches or mismatches of DO dynamics seize our attention: (1) the model performs very well before the liming and fertilization operation occurred; (2) the model's prediction overestimates the amplitude of the oscillation of the observations during the bloom, while constantly underestimates thereafter the bloom; (3) after the bloom the model's prediction shows a centric tendency and fails to follow the trend of the variation of the time series; (4) the highest DO concentration of the model's prediction lags that of the observations one cycle (24 hours).

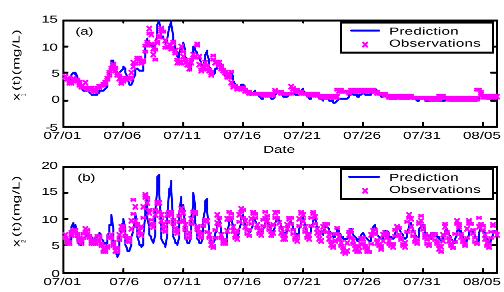

Figure 1. Recursive estimation results: One-step-ahead prediction vs. observations of (a) algal biomass and (b) dissolved oxygen.

As indicated in the introduction, these mismatches between the behavior of the model and system could be rooted in the failure of the *fixed* model formation to track the structural change of the *real* system. We may search for the possible explanations for the above observations via inspecting the successful recursive estimation of the parameters (both time invariant and *time variable*, shown in Figure 2), through which the model structure is formed. Obviously, the presumed time invariant parameters k_1 and k_2 stay stable for the rest of the period after the transient stages, while the decay rate of the total organic matter does not. This is not surprising because this first-order term is an extreme simplification for the consumption of the dissolved oxygen resulting from the degradation of all organic matter. Therefore, a more detailed description of the decomposition of organic matter is indispensable, for example, by classification of the organic matter and the associated decay processes. The increase in $k_5(t)$ - sources of DO other than reaeration and *algal* photosynthesis - suggests that there exist other processes contributing to DO concentration in the water column. During the operation of the pond experiment, duckweed, a species of floating macrophytes, grew very fast after the first fertilization. It started from the rim of the pond and eventually covered most of the surface. That the significant production and consumption of DO by the photosynthesis and respiration of the duckweed are not explicitly included in the simple model may cause the model's prediction always to underestimate the amplitude of the diurnal oscillation (referring to Figure 2). It is also worth mentioning that the significant changes of the elements in **K** matrix (shown in Figure 3) in early July give evidence of system change right after the implementation of liming and fertilization.

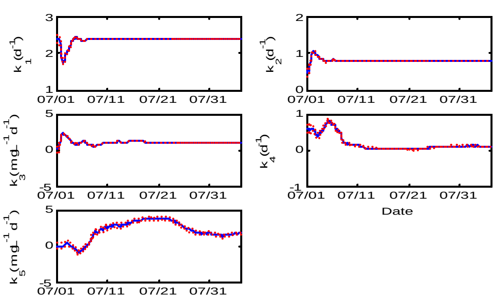

Figure 2. Recursive estimation results: estimates (solid line) and standard errors (dash line, almost invisible) of the time-invariant parameters (k_1, k_2, k_4) **and time-varying parameters** ($k_3(t)$**,** $k_5(t)$)**.**

CONCLUSIONS

A comprehensive data set obtained from an aquaculture pond with the assistance of the state-of-art water quality monitoring equipment (EPCL) allows the recursive parameter estimation for the algae-DO interaction model. The successful application of the modified RPE filter to the model and observations tells as that: (1) the pond system experienced a structural change in its behavior since the liming and first fertilization in early July; (2) the photosynthesis and respiration of the duckweed in the pond considerably affected the DO dynamics; and (3) a first-order decay reaction is inadequate to describe the degradation of the total organic matter in the pond system.

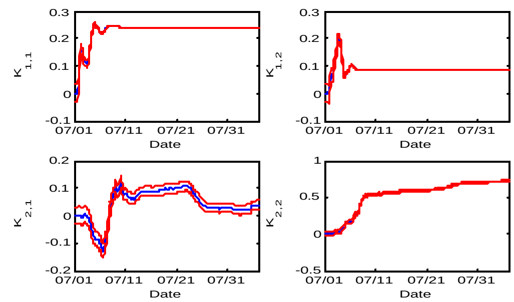

Figure 3. Recursive estimation results: estimates (solid line) and standard errors (dash line) of the elements of K matrix.

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