MODELING PHOSPHORUS DYNAMICS IN SHAGAWA LAKE

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I. Introduction

Most of the modeling done for ecological systems falls into one of two categories, each of which has a serious disadvantage. Large systems models contain numerous variables and parameters in attempts to maximize mechanistic realism. Because of their complexity and large parameter spaces, these models are difficult to corroborate with typically small ecological data bases. On the other hand, purely statistical models summarize data well but have little predictive value when ecosystem inputs or internal structures change. Occasionally, however, one studies a system whose dynamics can be described by a fairly simple mechanistic model and whose data base is large enough to permit statistical evaluations of model adequacy.

We encountered this situation in attempting to model the dynamics of phosphorus in a eutrophic lake. This paper describes the development and parameter estimation of a mass balance model for phosphorus. Sufficient data exists to statistically test the adequacy of the model, and we compare model projections with further data when phosphorus inputs to the lake are significantly reduced.

II. Background

Shagawa Lake, in northeastern Minnesota, has been intensively studied by the U.S. Environmental Protection Agency for many years. The lake has a long history of cultural eutrophication; in 1973, a tertiary wastewater treatment plant, funded by EPA and the City of Ely, MN, began operation in an attempt to reduce the supply of the critical nutrients that were considered responsible for recurrent algal blooms. Specifically, the plant was designed to remove a large proportion of the phosphorus (P) from wastewater effluent which fed into the lake.

Since 1973, the treatment plant has successfully kept supplies of P to Shagawa Lake at ~20% of their former levels. It was expected that, with reduced inputs of P to the lake, P concentrations would gradually decline as P was lost to outflow and to deposition into lake sediments, thus relieving the eutrophic condition.

A central objective of the continuing Shagawa study is to predict the dynamics of P levels in the lake. We would like to predict whether or not a steady-state condition will eventually occur if the reduction in P inputs is maintained. Assuming a steady state will be reached, we would also like to predict the length of time required to reach steady state, and whether steady-state P levels will be low enough to significantly reduce algal growth.

Detailed accounts of the wastewater treatment project and the limnology of the lake can be found in the following: Malueg et al. (1975); Larsen and Malueg (1976); Schults et al. (1976). Summaries of the dynamics of phosphorus and chlorophyll a in Shagawa are presented in Larsen et al. (1975) and Larsen et al. (1978a).

In conjunction with the long-term monitoring of chemical and biological characteristics of the lake, EPA researchers have worked with several models to describe Shagawa's history and predict its future trophic status. These models and their predictions have been fully described by Larsen and Mercier (1976).

The modeling effort described in this paper was, to some extent, motivated by Hsu's recent model study of Shagawa Lake (1976). Hsu treated the phosphorus (P) levels in the lake, recorded weekly between 1971 and 1975, as a time series. He recognized the recurring seasonal fluctuations seen in the pre-treatment data (Fig. 1) and described this pattern with two models. The first model was a stochastic auto-regressive moving-average equation (Box and Jenkins, 1970) which produces the recurrent seasonal pattern by requiring the P level at any given week in a year to be highly correlated with the P level in the same week of the previous year. In the second model, Hsu fit a deterministic model, consisting of piecewise linear and sinusoidal functions, to the pretreatment data, and then described the residual differences between model and data with a Box-Jenkins moving average model.

Both models gave an excellent fit to the pretreatment pattern of P concentrations. However, because they were both strictly empirical and based on 1971-1972 data, neither model could predict the downward trend in lake P levels which began following the start of wastewater treatment in 1973. Hsu was able to follow this trend by superimposing another deterministic component on one of the previous models, but the basic model inadequacy still remained. Purely empirical models cannot predict novel structural changes in a time series.

We recognized this problem in the empirical approach and decided to try a simple mechanistic deterministic model to describe the underlying seasonal fluctuations in lake P levels. However, we also saw the value of the time series techniques advocated by Hsu to deal with the residual differences between a deterministic model and data. We used time series methods to study the adequacy of a mechanistic P model and to provide confidence limits for the P trajectories which it would predict.

This paper describes the development of a mechanistic model and treats in some detail the estimation of model parameters, analysis of residuals, and generation of confidence intervals. The actual model predictions as compared with observed lake P levels and the resulting implications for recovery of the lake are discussed in another paper (Larsen et al., 1978a). Here the emphasis will be on the analytical methods which generated the model predictions and the limitations on these methods imposed by the data.

III. The Deterministic Model

We used a mass balance equation to describe changes in lake P. In the model, P is dealt with as a concentration by dividing mass flow rates by the lake volume. As illustrated by Figure 2, the change in P levels is a sum of inflow, outflow, deposition and sediment release rates.

$$\frac{d[P]}{dt} = \frac{J}{V} - \frac{Q}{V}[P] - \sigma_p[P] + \frac{R}{V} \qquad (1)$$

where: $[P]$ = Concentration of total P, (μg/l)

J = Rate of P supply from external sources

V = Lake volume

Q = Rate of water outflow

σ_p = Instantaneous loss rate of P to the lake sediments.

R = Rate of P release from the sediments

With the exception of the release term, $R/_V$, equation (1) is an accepted description of an instantly well-mixed lake system which loses P to the sediments (Vollenweider, 1975; Sonzogni et al., 1976; Larsen et al., 1978a).

Shagawa Lake is unusual in that its P dynamics have been dominated by a significant feedback of P from the sediments. This release of P appears in Figure 1 as the sudden increases which begin about the 10th and 25th weeks of each year. Larsen et al. (1978b) discuss the mechanisms for this phenomenon, and their analysis indicates that both the spring and summer releases begin suddenly, proceed at a constant rate for a number of weeks and then end suddenly. Thus, we modeled the release rate as

$$R(t) = \begin{cases} R_1, & t_1 < t \leq t_2 \\ R_2, & t_3 < t \leq t_4 \\ 0, & \text{otherwise} \end{cases} \qquad (2)$$

The switch times t_1 - t_4 refer to specific weeks of an arbitrary year, so R(t) is a periodic function having a period of 1 year. A final assumption in equation (1) is that we take σ_p to have one of two constant values depending on the season of the year, viz.

$$\sigma_p = \begin{cases} \sigma_p{}^s & \text{if lake is ice-free (week 17 to week 46)} \\ \sigma_p{}^w & \text{if lake is ice-covered (week 46 to week 17)} \end{cases}$$

This assumption is more in agreement with the mechanics of P deposition than the use of a fixed σ_p.

Equation (1) with a piecewise constant σ_p and R(t) specified by (2), constitutes the deterministic model for P in Shagawa Lake. The schedules for P input (J) and water flow rate (Q) are provided on a weekly basis from flow and P loading data whose measurement has been described elsewhere (Malueg et al., 1975; Larsen et al., 1975; Larsen and Malueg, 1976).

IV. Preliminary Model Analysis

Because equation (1) is linear we can address the questions of model steady-state behavior which we previously raised in section II with respect to actual lake dynamics. Suppose the model is started at an arbitrary initial condition. Further, suppose the same weekly schedules for J and Q are used in the model year after year so that all parameters and forcing functions are periodic with a period of 1 year. Then there exists a unique steady-state for [P(t)] which has the same period as that of the forcing function, J(t)/V + R(t), i.e. the steady state has a period of 1 year (Yakubovich and Starzhinskii, 1975). This result is true as long as the unforced model, with J(t)/V + R(t) = 0, has no periodic steady state. By a result of Floquet theory (D'Angelo, 1970), the unforced model can have a periodic steady state only if

$$\int_0^{1\ yr} \left[\frac{Q(t)}{V} + \sigma_p \right] dt = 0 \quad \text{(D'Angelo, 1970, p. 194)} \qquad (3)$$

Since Q and σ_p are not negative, the integral cannot be zero and the steady state is periodic in the forced model.

This steady-state result was borne out by simulations in which the initial condition for the model was taken to be the value of [P] at the end of 1972. Following parameter estimation, the model was run with a reduced

schedule for inputs typical of a post-treatment year and two different water flow schedules - one for a "wet" year and one for a "dry" year. In both cases, steady-state was reached within three years.

Thus, if the model is valid, we would expect to see the lake P levels show a new steady-state type of behavior within a few years after P inputs are reduced. Of course, an exact steady state will not be seen because of year-to-year variations in the loading and washout rates, J and Q.

V. Parameter Estimation

The next stage in the model development is the estimation of parameters for equation (1) based on the pretreatment data time series of Figure 1. For the estimation, the pretreatment interval from the onset of ice cover in late 1971 until the onset of ice cover in 1972 was partitioned into an ice-covered and an ice-free period. The 1971-1972 ice-covered interval (23 weeks) was used to estimate σ_p^w, R_1, t_1 and t_2; the ice-free period during 1972 (29 weeks) was used to estimate σ_p^s, R_2, t_3 and t_4. The remainder of the pretreatment period, made up of the first 46 weeks of 1971 and the last 6 weeks of 1972, was used to corroborate the model (Fig. 3).

We used a least-square criterion for the estimation, i.e.

$$\text{Minimize: } C = \sum_k ([P]_k^* - [P]_k)^2 \qquad (3)$$

with respect to the parameters σ_p^w, σ_p^s, R_1 R_2, t_1 t_2 t_3 t_4. In equation (3), $[P]_k^*$ and $[P]_k$ are weekly concentrations from the data and model, respectively, and the week index k runs over the appropriate estimation interval.

The large size of the parameter space strongly suggests using a directed search technique to minimize C. There are several gradient search algorithms

available for this type of optimization (Pierre, 1969), and we decided to use a gradient approach. However, the problem of minimizing C has an unusual feature -- the gradient of C must be computed with respect to the switch time parameters, t_1 - t_4.

Fortunately, methods which have been derived in the context of optimal control theory for calculating this type of gradient do exist. It is not difficult to recast the minimization problem (3) in control theoretic terms. We view equation (3) as a cost functional for a linear tracking problem with fixed initial and final times (Kirk, 1970).

In the remainder of this section we will sketch the results from the calculus of variations which compute the gradient of C. We follow closely the method of Hasdorff (1976), which should be consulted for derivations and other mathematical details. One preliminary note: the cost functional C will be restated as an integral to simplify the mathematics. Implementation of the results requires that discrete time be used, i.e., C takes the form of equation (3) and equation (1) is restated as a difference equation with an update interval of one week. However, since equation (1) is linear with rate coefficients having small absolute values, discretization of the continuous equations is straightforward and details will be omitted.

Let $\tilde{v} = [\sigma_p{}^w, R_1\ t_1, t_2]^+$, where the + denotes vector transpose and $\sim$ signifies a vector. For estimation of these parameters we restate C as

$$C = \int_{t_o}^{t_f} (x_1^* - x_1)^2\ dt \qquad (4)$$

where $[t_o, t_f]$ is the 1971-1972 ice-covered period, and where [P] has been renamed x_1. We also restate equation (1) as

$$\frac{dx_1}{dt} = f_1(\tilde{x}, \tilde{v})$$

with f_1 given by the right-hand side of equation (1) and $\tilde{x} = [x_1, x_2]^+$. Define the state variable $x_2(t)$ by

$$\frac{dx_2}{dt} = f_2(\tilde{x}, \tilde{v}) = (x_1^* - x_1)^2, \qquad x_2(t_0) = 0 \tag{5}$$

This definition allows us to write the cost functional in terms of a system state variable, viz.

$$C = \phi\,(\tilde{x}(t_f)) = x_2(t_f) \tag{6}$$

The notation combines the systems dynamical equation and the cost functional into a single state equation

$$\frac{d\tilde{x}}{dt} = \tilde{f}\,(\tilde{x}, \tilde{v}) \tag{7}$$

Finally, we need to define adjoint variables, $\tilde{\lambda}\,(t)$, also known as costate variables or Lagrange multipliers (Kirk, 1970). The adjoint variables satisfy the state equation

$$\frac{d\tilde{\lambda}}{dt} = -\tilde{f}_x^+\,\tilde{\lambda} : \tilde{\lambda}(t_f) = \nabla_x\,\phi(\tilde{x}(t_f)) \tag{8}$$

In equation (8), $\tilde{f}_x$ is the matrix of partial derivatives whose ij th element is given by

$$(\tilde{f}_x)_{ij} = \frac{\partial f_i}{\partial x_j}, \quad i,j = 1,2$$

Also, ∇_x signifies a gradient with respect to the vector $\tilde{x}$, i.e.

$$\nabla_x \phi(\tilde{x}(t_f)) = \left[\frac{\partial \phi(\tilde{x}(t_f))}{\partial x_1} , \frac{\partial \phi(\tilde{x}(t_f))}{\partial x_2} \right]^+$$

Armed with these definitions, Hasdorff uses variational methods to calculate the gradient of an arbitrary cost functional, $\phi(\tilde{x}(t_f))$, with respect to several forms of initial conditions and input and control parameters. For the system described by equations (4) and (5) the gradient is

$$g(\sigma_p^w, R_1, t_1, t_2) = \begin{bmatrix} \int_{t_o}^{t_f} f_a^+ \tilde{\lambda}(t)dt \\ \int_{t_1}^{t_2} f_b^+ \tilde{\lambda}(t)dt \\ \tilde{\lambda}^+(t_1) \left[\tilde{f}(\tilde{x}(t_1),0) - \tilde{f}(\tilde{x}(t_1),R_1) \right] \\ \tilde{\lambda}^+(t_2) \left[\tilde{f}(\tilde{x}(t_2),R_1) - \tilde{f}(\tilde{x}(t_2),R_2) \right] \end{bmatrix} \qquad (9)$$

Each component in the gradient vector corresponds to the parameter having the same position in the argument list of g. In addition,

$$\tilde{f}_a^+ = \left[\frac{\partial f_1}{\partial \sigma_p^w}, \frac{\partial f_2}{\partial \sigma_p^w} \right]^+ \qquad \tilde{f}_b^+ = \left[\frac{\partial f_1}{\partial R_1}, \frac{\partial f_2}{\partial R_1} \right]^+$$

Calculation of the gradient is accomplished with the following sequence:

1. Given an initial guess for the parameter vector, $\tilde{v}$, the state equation (7) is integrated numerically from t_o to t_f. This calculation also gives the value of C.

2. The final state, $\tilde{x}(t_f)$, provides the initial condition for the adjoint equations via (8).
3. The adjoint system (8) is integrated backwards in time from t_f to t_o and the values of $\tilde{\lambda}(t)$ are stored.
4. Equation (9) uses the stored values of $\tilde{\lambda}(t)$ to compute the gradient g.
5. The values of C and g are passed on to a gradient search algorithm which uses them to change the parameter vector such that C decreases.

The sequence is repeated until C has been satisfactorily minimized. For step 5 of the sequence, we used the fast and efficient Davidon-Fletcher-Powell conjugate descent algorithm (Pierre, 1969). The algorithm is implemented by subroutines FMFP and DFMFP of the IBM System/360 Scientific Subroutine package. The algorithm converged quickly for this problem, but, due to the the noise in the data, the cost functional was fairly insensitive to small changes in some parameters. Thus, estimation runs were made in groups, with each run of a group having different initial guesses for the parameters.

Table 1 gives the best estimates for the model parameters. The fitted model and data are shown in Figure 3. As measured by the sum of squared residuals, the model showed a 25% better fit during the corroboration interval than it did during the estimation interval. Therefore we concluded that equations (1) and (2) with the parameter estimates of Table 1 provide an adequate deterministic model for the P dynamics seen in Figure 1.

VI. Analysis of Residuals

A. The Stochastic Model

The process of parameter estimation produced a "best fit" model according

to the least squares criterion. However, this type of fitting does not necessarily eliminate systematic departures, through time, between model and data. We can test for these trends by analyzing the model residuals using the time series techniques of Box and Jenkins (1970).

The residual time series e_k for 1971-1972 is shown in Figure 4. The first step in the analysis of this series is calculation of the mean and variance. Since the mean value of the series is effectively zero, we next studied the autocorrelation structure of e_k. The theoretical autocorrelation function at time lag j is defined by

$$\rho_j = \frac{E\,[(e_k - \mu_e)(e_{k+j} - \mu_e)]}{\sigma_e^2} \qquad (10)$$

where E is the expectation operator, j and k are discrete time indices, and μ_e and σ_e^2 are the mean and variance, respectively, of the series e_k.

Figure 5 shows the function ρ_j as estimated for the e's of Figure 4. The estimated values of ρ_j indicate whether the e-series is covariance stationary. If the e-series is stationary, then ρ_j will approach zero rapidly with increasing j. The dashed lines in Figure 5 show the standard error of the estimate of ρ_j. Estimated values of an autocorrelation which is theoretically zero are approximately normally distributed. Hence values of ρ_j, such as ρ_{17}, which are theoretically zero but fall outside the line have about a one-third probability of occurring (Box and Jenkins, 1970, p. 178).

Another restriction on the reliability of ρ_j estimates is provided by N, the number of data points available. Here N = 104, and Box and Jenkins (1970, p. 33) claim that estimates of ρ_j are unreliable for $j > N/4$. The deterministic model and the lake P dynamics operate on a fundamental period

of 1 year, so we expect to see a peak in ρ_j at $j = 52$. This peak does appear in Figure 5, but the above criterion requires at least 4 years of data for one to be statistically assured of its importance. As it is, we cannot depend on the estimated value of ρ_j beyond lag 26.

Based on Figure 5, we decided to try a stationary model for e_k with a theoretical autocorrelation function which is effectively zero beyond lag 2. A second order moving-average model of the following form is indicated:

$$e_k = a_k - \theta_1 a_{k-1} - \theta_2 a_{k-2} \qquad (11)$$

In equation (11), the a's are independent random shocks having zero mean and constant variance σ_a^2.

The model (11) was fit to the series e_k using an estimation algorithm given in chapter 7 of Box and Jenkins (1970). The results of the estimation produced

$$e_k = a_k + 0.55\, a_{k-1} + 0.2\, a_{k-2},\ \sigma_a^2 = 30.6 \qquad (12)$$

Finally, we apply diagnostic checks to assess the adequacy of the model (12). The procedure is to use (12) and the residuals e_k to generate a series a_k. If equation (12) is adequate, the a_k's should be uncorrelated with a zero mean. A white noise test is performed on the autocorrelation function of the a_k's (Box and Jenkins, 1970, p. 299). This test confirmed the adequacy of (12).

The preceding analysis shows that the model residuals, e_k, can be described by a stationary, random time series with a zero mean and a low order of autocorrelation. We interpret this result to mean that the mass balance model (1) adequately represents all of the deterministic information about P dynamics which can be extracted from the 1971-1972 data.

B. Forecasts and Confidence Limits

With the aid of equation (12) we can place confidence limits on the predictions of the deterministic model (1). We assume that the nature of the random errors, e_k, remains unchanged following the start of wastewater treatment in 1973. Following the method of Box and Jenkins (1970 chapter 5), we forecast values for the series e_k and superimpose the forecast on the deterministic predictions. The error variance of the forecast gives confidence limits for the prediction of e_k.

Let e_{k+j} = forecast of the e-series for j weeks ahead of the time origin k. If we take k as the last week in 1972, then, except for the first two weeks in 1973, the forecasts e_{k+j} are identically zero, since $\mu_e = 0$ and the model (12) is stationary. Therefore, the expected future value of the residuals is zero, and we center the confidence limits on the trajectory of the deterministic model.

For $j \geq 3$, the confidence intervals are defined by

$$\left[\begin{array}{l}\text{95\% confidence interval} \\ \text{at lead time j}\end{array}\right] = \hat{P}_{k+j} \pm U_{0.05/2} \cdot \sigma_e \qquad (13)$$

where $\hat{P}_{k+j}$ is the deterministic prediction at time k+j, and $U_{\varepsilon/2}$ is the deviate exceeded by the fraction $\varepsilon/2$ of the unit Normal distribution.

VII. Model Predictions

Figures 6 and 7 show model predictions compared with data for 1973-74 and 1975-76. The two predicted trajectories employ observed flow rates during 1973-1976 for the parameters Q(t). The prediction which assumes

treatment uses the observed P inputs for J(t), which are about 80% lower than pretreatment inputs (Larsen et. al., 1978a). We made the prediction which assumes no treatment by employing the average P input rate observed during the two pretreatment years 1971-1972. Confidence intervals are shown centered on the trajectory which assumes treatment, but intervals of equal width would also apply to the "no treatment" curve.

Since observed values for J and Q were used, Figures 6 and 7 are not predictions in the truest sense. To make such predictions, we would also need to forecast time series for J and Q, both of which are functions of river discharge, and thus of weather patterns. However, we compared simulations of the model which employed Q(t) for a typical "high" water year as opposed to a "low" water year and found that the P trajectories were never separated by more than 4 μg/l. Based on this trial, we feel that the model would provide good predictions for future normal water years.

The observed lake P response to reduced loading appears to be delayed since it follows the "no treatment" prediction more closely than the "treatment" prediction during most of 1973. However, by 1975 and certainly 1976, the observed lake P levels track the "treatment" prediction quite closely and consistently fall within the confidence intervals. Following a sharp reduction in P inputs, equations (1), (2) and (12) clearly provided an accurate description of P dynamics in Shagawa once the lake response has become stabilized. Larsen et al. (1978a) give a statistical summary of the results shown in Figures 6 and 7 and they discuss the Figures' implications for improvement in the trophic status of the lake.

VIII. Summary and Conclusions

We have outlined the methodology used to develop a predictive model of phosphorus dynamics in Shagawa Lake. The modeling process involved a sequence of steps, beginning with selection of a simple mass balance equation and mathematical formulation of the various rate functions in the equation. In the next stage, we estimated model parameters using a least squares criterion applied to pretreatment data of 1971-1972. The fitted model was then subjected to a time series analysis of its residuals to uncover systematic departures from the data. Upon finding no trends in the residuals, we judged the deterministic model to be adequate and went on to generate confidence limits from the stochastic model of the residuals. Finally, we made predictions of P levels for 1973-1976 and compared them with data.

In constructing this model we have taken an approach more akin to conventional statistics than to currently popular practices of systems ecology. That is, we began with the constraints imposed by the data base, constraints of sampling frequency, sampling duration, and types of variables sampled. Our goal was to build a predictive model which could extract the maximum amount of information about lake P dynamics from the available data, and would require as few assumptions about mechanisms or parameter values as possible. The recent work of Walker (1977) is an excellent discussion of this approach applied to a variety of lake water quality models.

The data base for Shagawa Lake constitutes one of the longest, most comprehensive records available for variables pertinent to algal-nutrient dynamics. Thus, even though equation (1) appears fairly elementary, it may be the most sophisticated model of its type which can be supported by currently available data.

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TABLE 1. Parameter estimates for equations (1) and (2)

Ice-covered season	Ice-free season
$\sigma_p^w = 0.035\ wk^{-1}$	$\sigma_p^s = 0.072\ wk^{-1}$
$R_1 = 280$ kg/wk	$R_2 = 500$ kg/wk
$t_1 =$ week 12	$t_3 =$ week 25
$t_2 =$ week 14	$t_4 =$ week 34

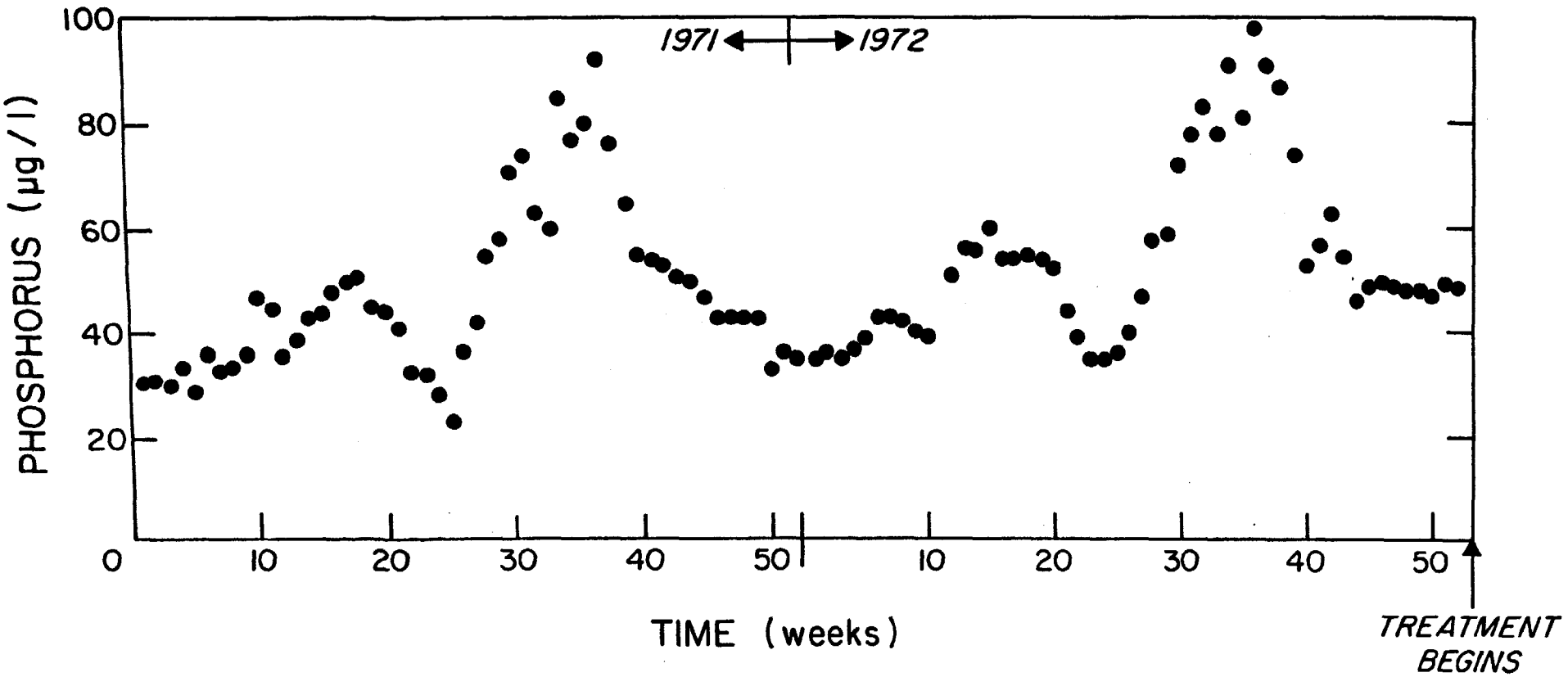

Figure 1. Weekly average total phosphorus levels in Shagawa Lake, 1971-1972.

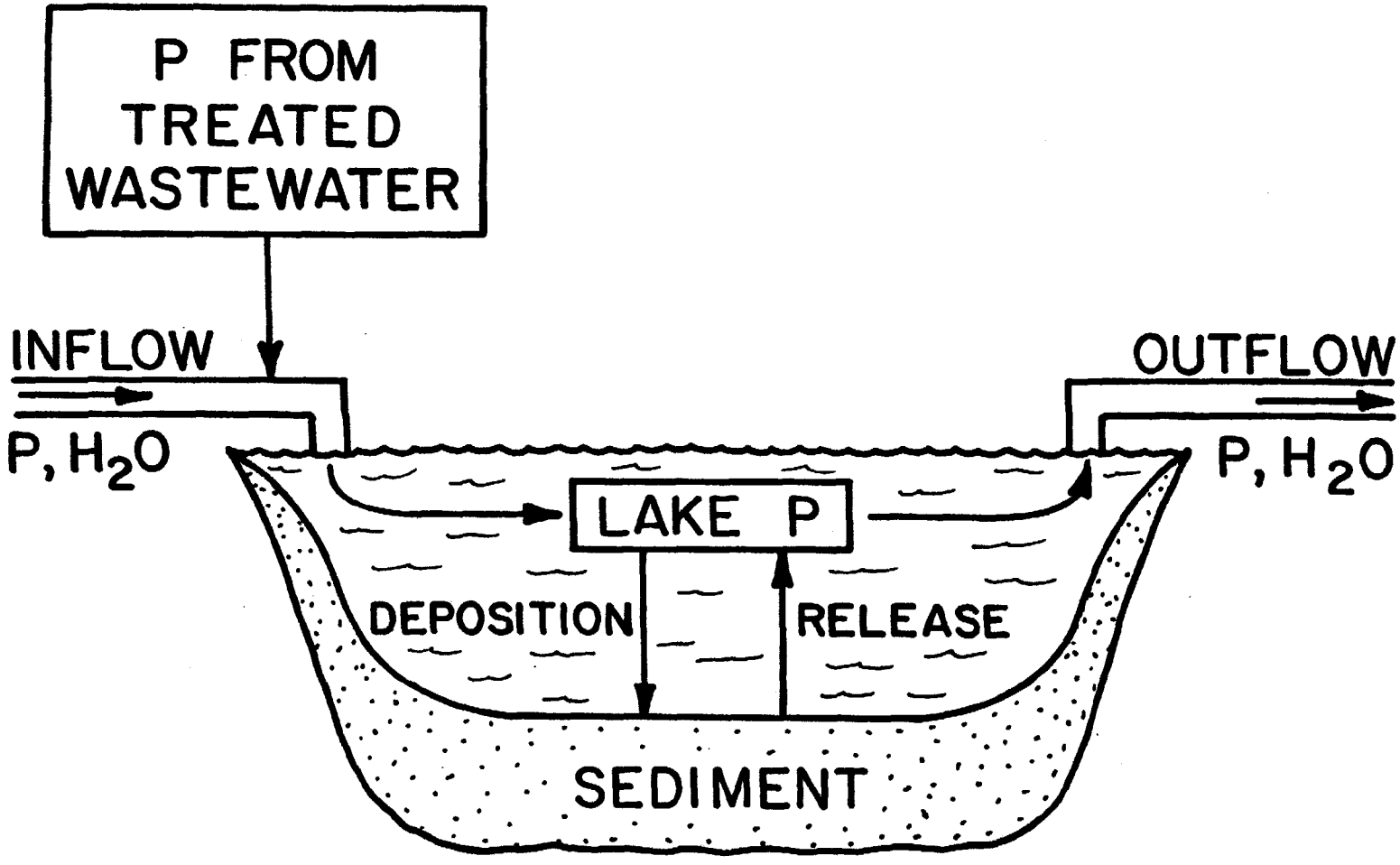

Figure 2. Sources and losses of phosphorus in Shagawa Lake.

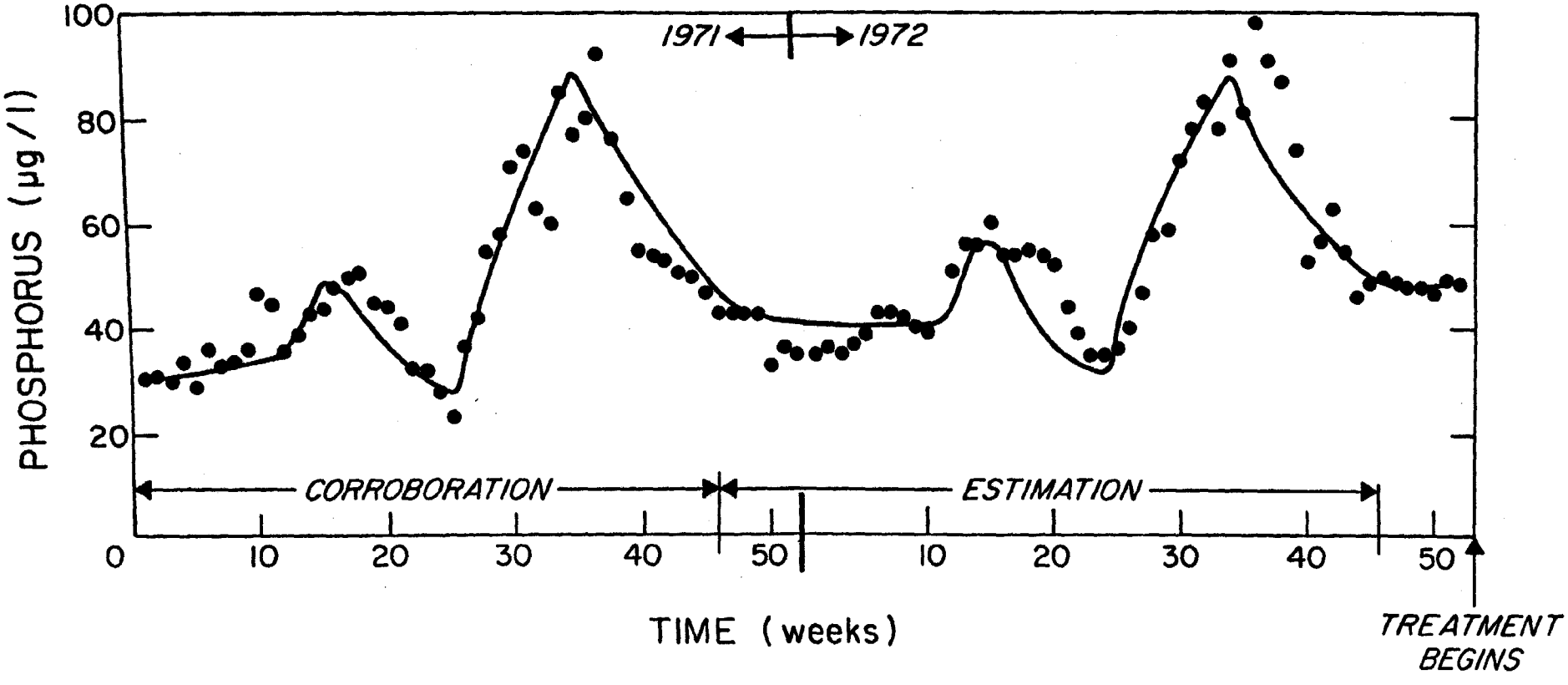

Figure 3. Fitted model trajectory, 1971-1972.

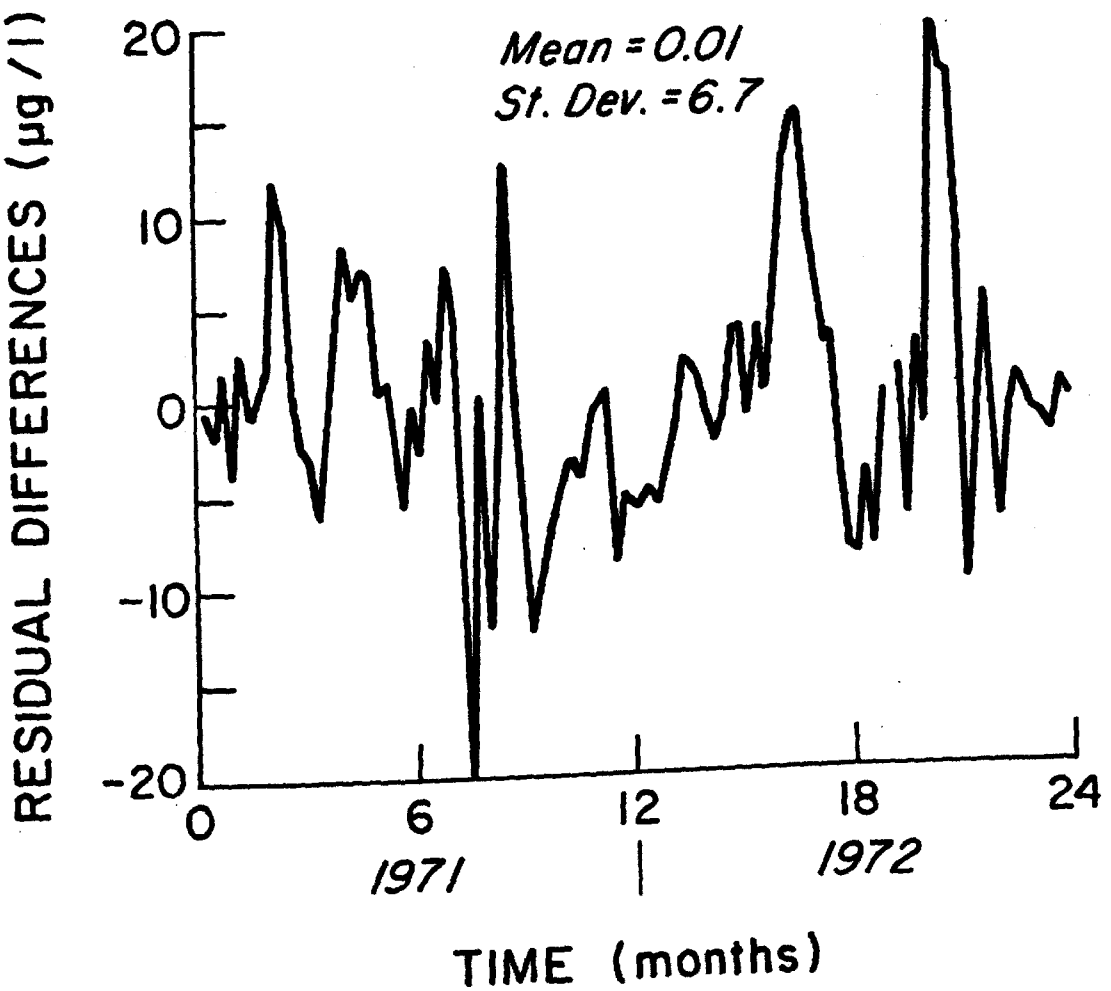

Figure 4. Weekly residual differences, $e_k = ([P]_k^{Data} - [P]_k^{Model})$, 1971-1972.

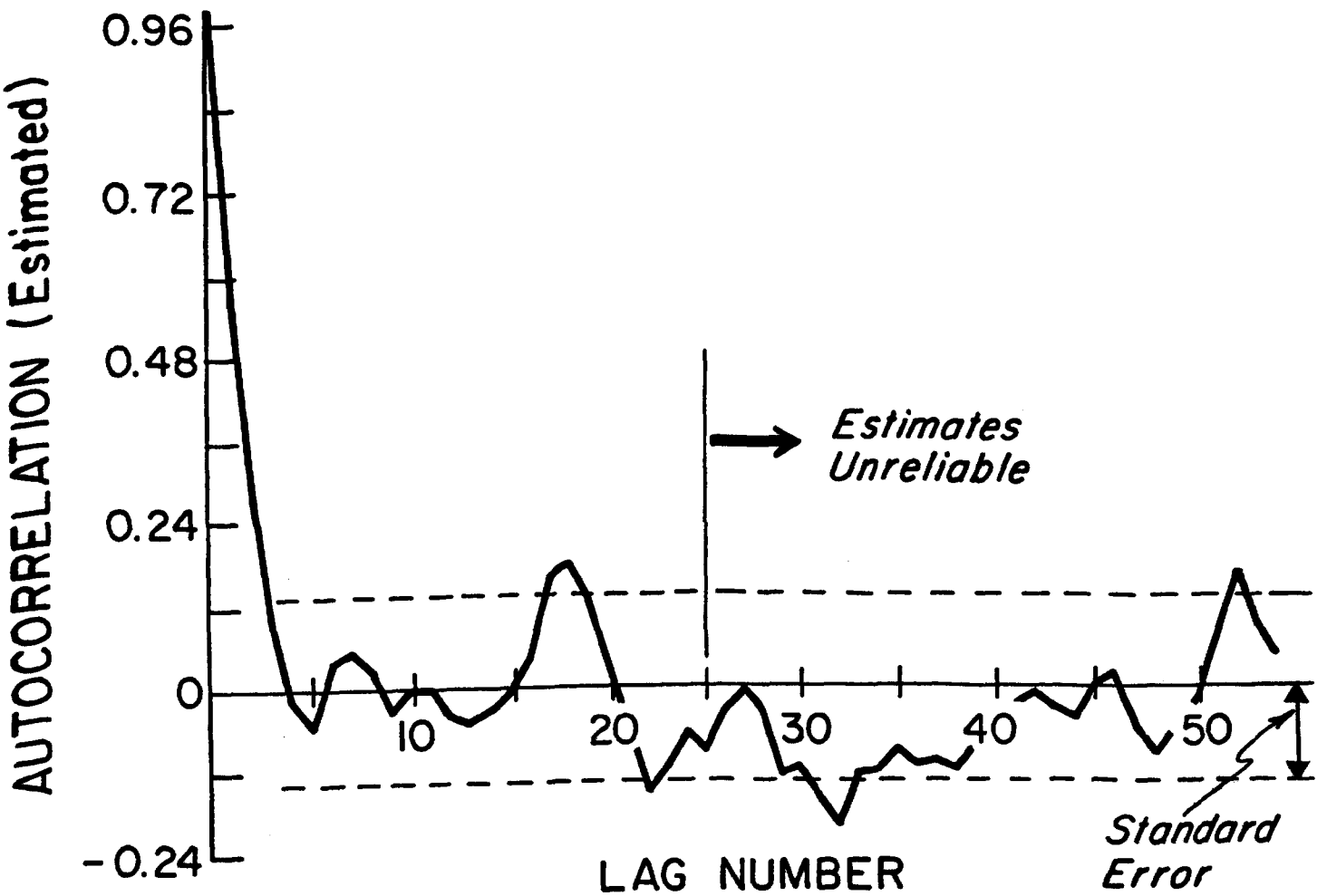

Figure 5. Autocorrelation of residual series.

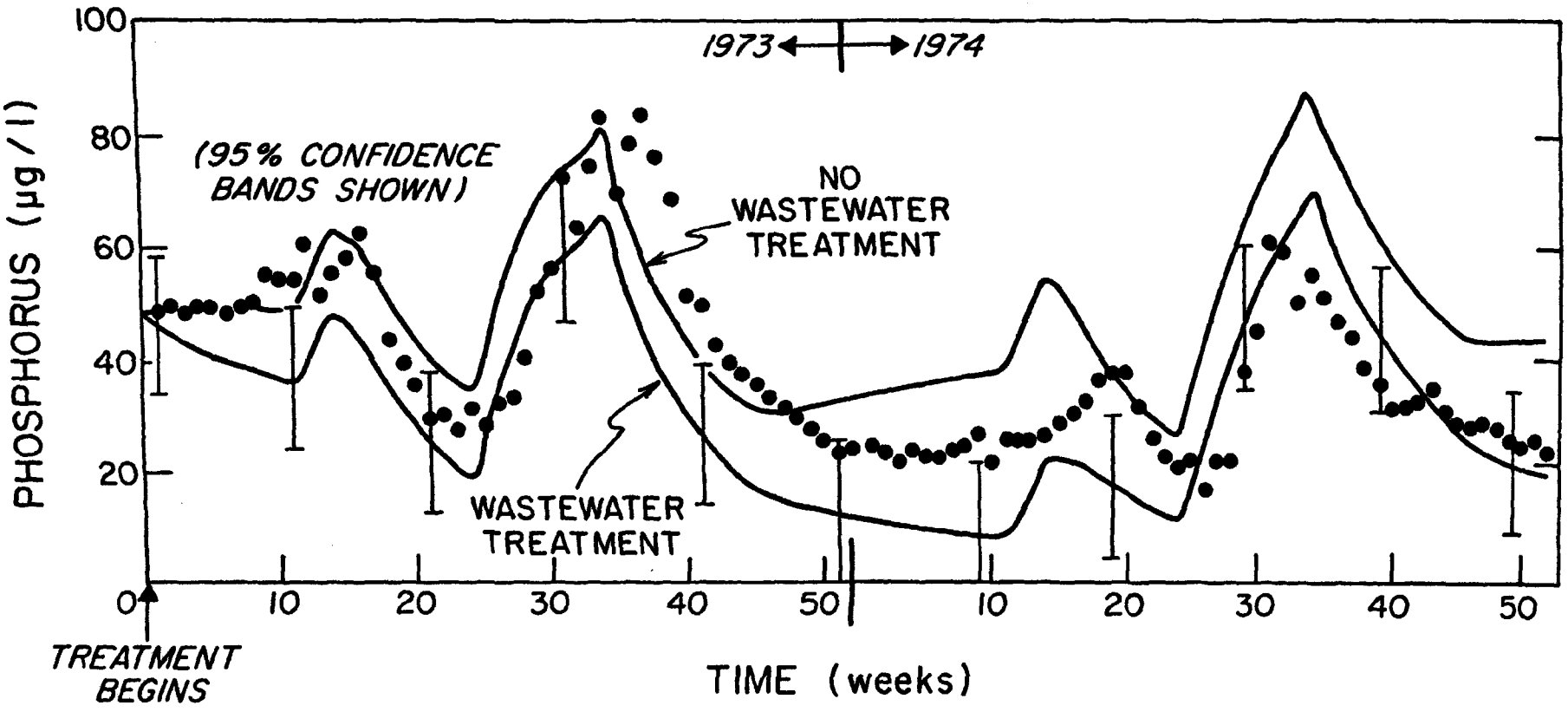

Figure 6. Model predictions compared with data, 1973-1974.

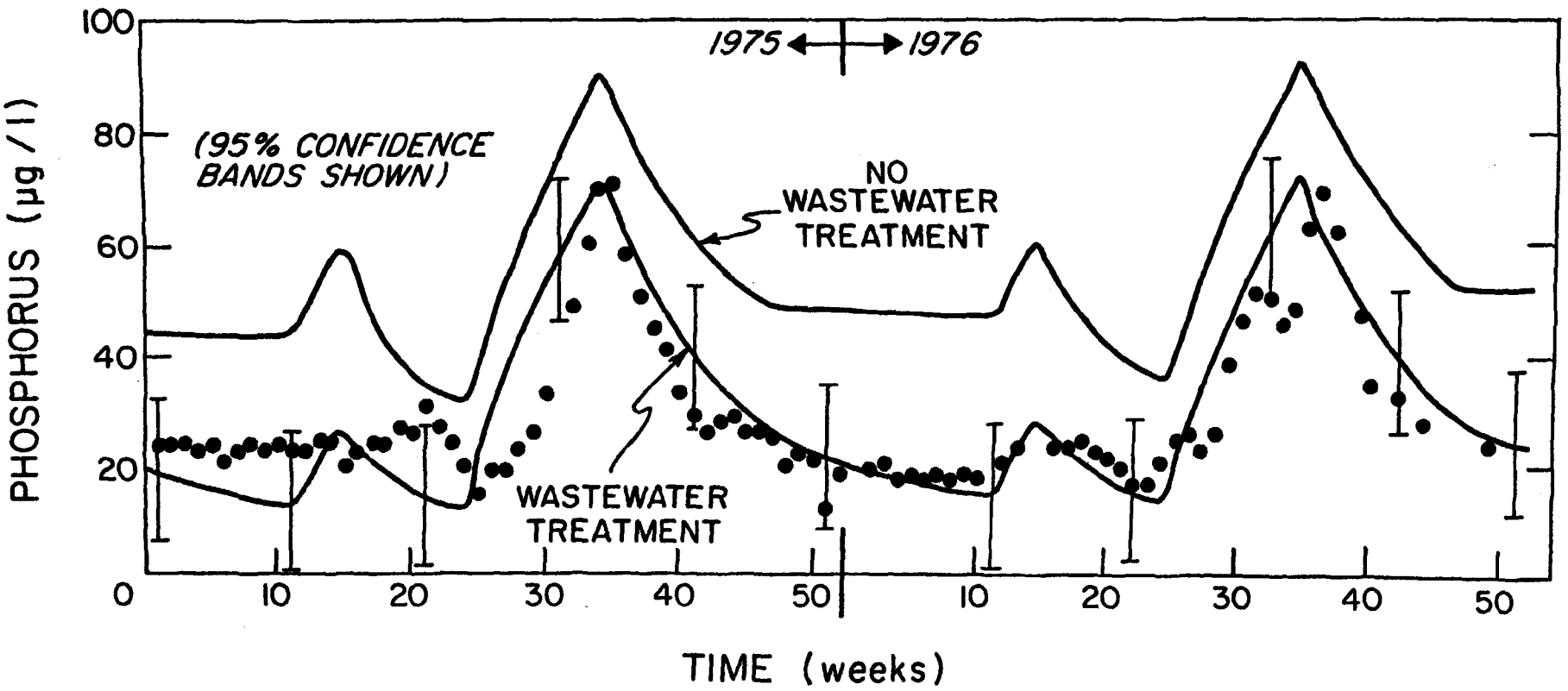

Figure 7. Model predictions compared with data, 1975-1976.