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METHODS FOR IMPROVING THE EFFICIENCY OF CALIBRATION OF A MODEL OF PHOSPHORUS CYCLING IN A LAKE ECOSYSTEM

ABSTRACT: As has been indicated by practice, the traditional trial and error method is not an efficient tool for estimating the parameters of ecological models. The degree of complication of a typical ecological model also makes it impossible to use available formal algorithms. Two techniques can, however, be suggested which considerably improve the process of parameter estimation. One of them is the method of step by step merging subsequent state equations, and the other that of aiding the estimation process with sensitivity analysis.

KEY WORDS: phosphorus cycling, lake modelling, parameter estimation, sensitivity analysis.

1. INTRODUCTION

If the nature of the processes going on in an ecosystem, and the relations among ecosystem elements are known well, the way of mathematical representation of information and formulation of the equations of a model is a compromise between the tendency towards a true description of the phenomena that occur and the need to simplify the model. Most important is the adjustment of the structure of the model and the description method used in it to the aim of the model.

For this reason, in model equations descriptions in the form of functions are used which define complex processes only in a simplified way. The parameters used in the function often represent quantities whose values cannot be obtained by field measurement or laboratory experiments. In this case the only solution on which the construction of a model can be based is the estimation of its parameters. When performing the estimation, it is necessary to take into account parameter value ranges,

where these ranges are known, at the same time allowing a certain degree of freedom in the determination of the remaining parameters of which even approximate values are not known.

The trial and error method, routinely applied to parameter estimation, does not enable the modeller to determine whether the cause of existing discrepancies between simulation results and the behaviour of a real system is a fault in the structure of the model itself or inadequate determination of parameter values.

In spite of their being sometimes applied to ecological models (L e w i s and N i r 1978, B e n s o n 1979, J ø r g e n s e n et al. 1981), the use of formal procedures for parameter estimation is fairly limited on account of the rapidly growing, with the number of parameters, dimensionality of the error function minimization task.

The trial and error method ensures a greater flexibility of action for the modeller than to formal techniques. But, like them, it does not make it possible to verify the structure of the model.

The aim of this study was to analyse the problems associated with the estimation of the parameters of an ecological model and consider the use of some methods to improve the efficiency of model calibration.

2. THE MODEL

Problems related to ecological model parameter estimation were analysed on the basis of a model of phosphorus cycling in the epilimnion ecosystem of Lake Głębokie (for detailed description of the model see U c h m a ń s k i 1988). Parameter

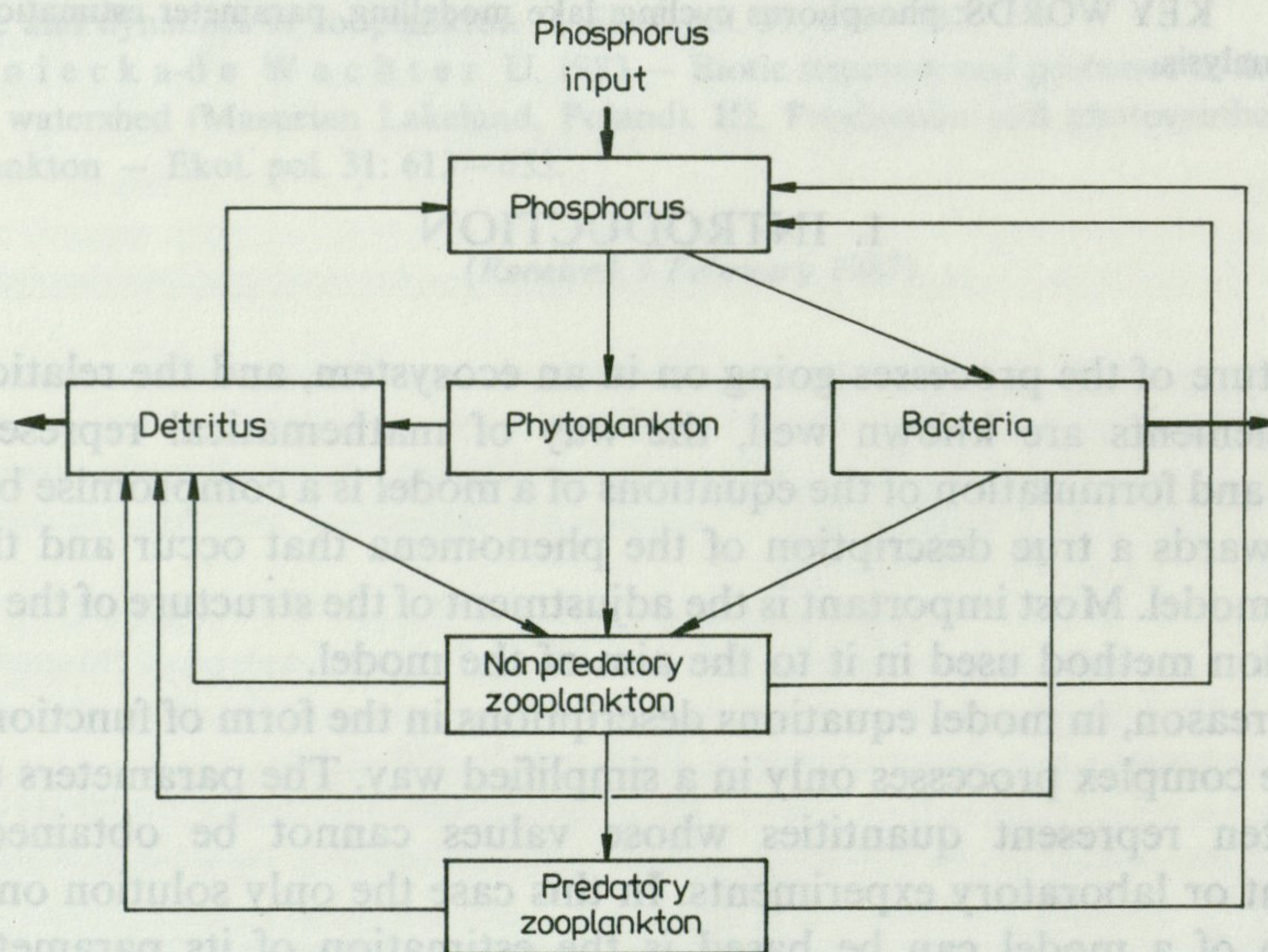


Fig. 1. A block diagram of the model of phosphorus cycle in the epilimnion of Lake Głębokie

estimation problems of this model are typical of a large class of ecological models. A diagram of the model considered has been presented in Figure 1.

The model describes the dynamics of six variables – the concentrations of: orthophosphate phosphorus $P-PO_4$, bacteria, phytoplankton, nonpredatory and predatory zooplankton and detritus. All the variables are expressed in $\mu\text{g P}\cdot\text{l}^{-1}$ units. The epilimnion ecosystem of Lake Głębokie is supplied with phosphorus from sources outside the lake and from its deeper layers. The mineral phosphorus pool can be utilized directly by bacteria and phytoplankton. They are the source of this nutrient for the next trophic level represented by nonpredatory zooplankton. Another source of food, for nonpredatory zooplankton, is, besides phytoplankton and bacteria, the

Table 1. Equations of the model

P – phosphorus, F – phytoplankton, B – bacteria, D – detritus, Z_{np} – nonpredatory zooplankton, Z_p – predatory zooplankton, I – light intensity, T – temperature. Definitions of parameters see Table 3

$$\frac{dZ_p}{dt} = G_{zp}^{\max} F_z^1(T) F_{zp}^2(Z_{np}) A_{zp} Z_{np} - Q_{zp} - M_{zp}$$

$$\frac{dZ_{np}}{dt} = G_{znp}^{\max} F_z^1(T) F_{znp}^2(F, B, D) A_{znp} Z_{np} - G_{zp} - Q_{znp} - M_{znp}$$

$$\frac{dF}{dt} = G_f^{\max} F_f^1(T) F_f^2(I) F_f^3(P) F - G_{znp}^{\max} F_z^1(T) c_1 f_{znp}^1(F) Z_{np} - Q_f - M_f - G_b^{\max} F_b^1(T) F_b^2(D) F_b^3(P) B$$

$$\frac{dB}{dt} = G_b^{\max} F_b^1(T) F_b^2(D) F_b^3(P) B - G_{znp}^{\max} F_z^1(T) c_2 f_{znp}^2(B) Z_{np} - S_b - S_b^{\text{sed}}$$

$$\begin{aligned} \frac{dD}{dt} = & S_f + S_b + S_{znp} + S_{zp} + (1 - A_{znp}) G_{znp} Z_{np} + (1 - A_{zp}) G_{zp} Z_p - G_{znp}^{\max} F_z^1(T) c_3 f_{znp}^3(D) Z_{np} - \\ & - G_d F_d^1(T) F_d^2(D) B - S_{\text{det}} \end{aligned}$$

$$\frac{dP}{dt} = \text{INFOS} + Q_{zp} + Q_{znp} + Q_b - G_f F - S_p$$

$$G_{zp} = G_{zp}^{\max} F_z^1(T) F_{zp}^2(Z_{np}) A_{zp} Z_{np}$$

$$F_z^1(T) = \exp(-v_z(T_z^{\text{opt}} - T)^2), F_f^1(T) = \exp(-v_f(T_f^{\text{opt}} - T)^2),$$

$$F_b^1(T) = \exp(-v_b(T_b^{\text{opt}} - T)^2),$$

$$F_b^2(P) = P/(g_2 B + P), F_b^3(D) = D/(g_1 B + D), F_d^2(D) = D/(K_d + D)$$

$$F_f^2(I) = (I/I_{\text{opt}}) \exp(1 - I/I_{\text{opt}}), F_f^3(P) = P/(K_f + P)$$

$$F_{zp}^2(Z_{np}) = 1 - \exp(-K_p Z_{np}), F_{znp}^2(F, B, D) = c_1 f_{znp}^1(F) + c_2 f_{znp}^2(B) + c_3 f_{znp}^3(D)$$

$$f_{znp}^1(F) = 1 - \exp(-K_n^1 F), f_{znp}^2(B) = 1 - \exp(-K_n^2 B), f_{znp}^3(D) = 1 - \exp(-K_n^3 D)$$

$$Q_{zp} = q_{zp} F_z^1(T) Z_p, Q_{znp} = q_{znp} F_z^1(T) Z_{np}$$

$$M_{zp} = m_{zp} Z_p, M_{znp} = m_{znp} Z_{np}, M_f = m_f F, M_b = m_b B$$

$$S_{\text{det}} = s_{\text{det}} D, S_b = s_{\text{det}} m B$$

detritus. The last link of the food chain in the ecosystem considered is the predatory zooplankton feeding exclusively on the nonpredatory zooplankton. The excretion of both zooplankton groups contributes to a partial renewal of the phosphorus pool. The death of the living elements of the ecosystem causes an increase in the amount of detritus. The detritus pool is additionally supplied with the part of zooplankton food that is expelled as faeces. The phosphorus contained in the detritus is partly released into the environment owing to bacterial decomposition. The sedimentation of bacteria-inhabited detritus particles is equivalent to their output from the system.

The model consists of six ordinary nonlinear differential equations (see Table 1). It is supplemented with driving functions that define changes in: temperature, light intensity and input of mineral phosphorus to the system (Table 2).

Table 2. Driving functions applied in the model

t — time, E — light extinction coefficient, z — depth. Definitions of parameters see Table 3

Epilimnion depth:

$$z_{epi} = P_2(0.000467 t^2 - 0.1623278 t + 17.52975)$$

Epilimnion temperature:

$$T = 8 - 12 \cos(2\pi(t - 25)/365)$$

Light intensity:

$$I = P_3(1046 - 1004.16 \cos(2\pi(t - 5)/365)) \exp(-Ez)$$

Phosphorus input:

$$INFOS = P_1(-170.9751 + 4.2469t - 0.298t^2 + 0.821 \cdot 10^{-5}t^3 - 0.773 \cdot 10^{-7}t^4)$$

There are a total of 33 parameters in the equations of the model (Table 3). Some of them are of commonly known biological meaning, others are empirical quantities introduced into the model along with simplification functions used for the definition. As example parameters, well defined biologically, the following can be given: optimum temperatures for the growth of the phyto- and zooplankton, mortality rates, food-assimilation coefficients, optimum light intensity for photosynthesis, while the so-called Ivlev parameters are examples of entirely empirical quantities. Parameters g_1 and g_2 , present in the bacterial-concentration dynamics equation, are of similar meaning. The products of their multiplication by the state variable, $g_1 \cdot B$ and $g_2 \cdot B$, can be interpreted as the half-saturation constant in the Michaelis-Menten model.

To solve the differential equations of the model, the Runge-Kutta six-order method was used with a one-day time step. Because for the assessment of the adjustment of the simulation results to the real behaviour of the system a subjective criterion was used, it was convenient to graphically present the simulation results in common graphs with the measured values.

Table 3. Designations of parameters present in the model

P_1	— coefficient of phosphorus input to the system
$S_p(\text{day}^{-1})$	— phosphorus sedimentation rate
$G_f^{\max}(\mu\text{g P} \cdot \text{l}^{-1} \cdot \text{day}^{-1})$	— maximum rate of phytoplankton increase
$K(\mu\text{g P} \cdot \text{l}^{-1})$	— half-saturation constant for phytoplankton
P_2	— epilimnion depth coefficient
$I_{\text{opt}}(\text{J}(\text{cm} \cdot \text{day})^{-1})$	— optimum light intensity for phytoplankton
P_3	— light intensity coefficient
$T_f^{\text{opt}}(^{\circ}\text{C})$	— optimum temperature for phytoplankton
V_f	— temperature coefficient for phytoplankton
$m_f(\text{day}^{-1})$	— phytoplankton mortality rate
$G_f^{\max}(\mu\text{g P} \cdot \text{l}^{-1} \cdot \text{day}^{-1})$	— maximum growth of nonpredatory zooplankton
C_1	— maximum proportion of phytoplankton in the diet of nonpredatory zooplankton
C_2	— maximum percentage of bacteria in the diet of nonpredatory zooplankton
C_3	— maximum percentage of detritus in the diet of nonpredatory zooplankton
$K_n^1(\text{l} \cdot \mu\text{g P}^{-1})$	— Ivlev parameter for phytoplankton as food
$K_n^2(\text{l} \cdot \mu\text{g P}^{-1})$	— Ivlev parameter for bacteria as food
$K_n^3(\text{l} \cdot \mu\text{g P}^{-1})$	— Ivlev parameter for detritus as food
$T_z^{\text{opt}}(^{\circ}\text{C})$	— optimum temperature for zooplankton
V_z	— temperature coefficient for nonpredatory zooplankton
A_{znp}	— assimilation coefficient for nonpredatory zooplankton
$q_{znp}(\text{day}^{-1})$	— excretion coefficient for nonpredatory zooplankton
$m_{znp}(\text{day}^{-1})$	— nonpredatory zooplankton mortality rate
$G_{znp}^{\max}(\mu\text{g P} \cdot \text{l}^{-1} \cdot \text{day}^{-1})$	— maximum growth of predatory zooplankton
$K_p(\text{l} \cdot \mu\text{g P}^{-1})$	— Ivlev parameter
A_{zp}	— assimilation coefficient for predatory zooplankton
$q_{zp}(\text{day}^{-1})$	— excretion coefficient for predatory zooplankton
$m_{zp}(\text{day}^{-1})$	— predatory zooplankton mortality rate
$G_b^{\max}(\mu\text{g P} \cdot \text{l}^{-1} \cdot \text{day}^{-1})$	— maximum growth rate of bacteria
g_1	— parameter in the equation for bacteria
$m_b(\text{day}^{-1})$	— mortality rate for bacteria
m	— degree of detritus colonization by bacteria
$T^{\text{opt}}(^{\circ}\text{C})$	— optimum temperature for bacteria
g_2	— parameter in the equation for bacteria
$S_{\text{det}}(\text{day}^{-1})$	— detritus sedimentation rate
$K_d(\mu\text{g P} \cdot \text{l}^{-1})$	— half-saturation constant for bacterial decomposition of detritus
C_d	— parameter in the equation for detritus

3. A TRIAL FOR ESTIMATING MODEL PARAMETERS WITH TRADITIONAL METHODS

One of the theoretically possible estimation methods is the use of the so-called formal method. It requires first of all a measure, called the estimator, to be defined. The measure makes it possible to compare the dynamics of the simulated state variables with the real responses of a modelled object represent by measurement data. The most frequently used among many estimators is the least-squares estimator (e.g. R i n a l d i et al. 1979).

$$\min_p \left(\sum_{i=1}^m \sum_{j=1}^n (x_{ij}(t, p) - x_z)^2 \right)$$

where: n — number of state variables, m — number of state-variable measurements, p — vector of parameters, x_z — measured value of the i -th state variable at a point of time corresponding to the j -th measurement, t — time.

In this case the parameter estimation process is equivalent to the solution of a nonlinear programming problem, that is, seeking the parameter values of the model for which the condition of error function minimization, defined as the total of squared deviations, has been satisfied. The possibility of using this method is, however, limited. If the above problems are processed on a modern computer, one can hope for a successful calculation only in those cases where at the most between ten and twenty parameters are being estimated. Even for relatively simple linear models the long processing time is very cumbersome. The cause of this is the complex form of the error function, as well as the sensitivity of the minimization algorithms to the initial approximation of the parameter values (K r a s z e w s k i 1982). Another drawback of this method is that all partial error functions are usually treated in the same way. In cases similar to that which occurred in the model considered in this study, where the value attained by the concentration of bacteria was several-dozen times higher than the level of detritus concentration, partial error functions (for particular state variables) with differing weights should be taken into account. The parameter values obtained by this method satisfy the minimum function error criterion, but they are often rejected by ecologists because they do not agree with the accepted biological interpretations. In view of the above disadvantages and restrictions of the formal method, investigators usually decide not to use the algorithms it proposes, and to use the possibility of subjective evaluation of the adjustment of successive simulation results to measurement data obtained by the trial and error method.

In the method the assumption is made that the values of most parameters are known and need not be estimated. The object on which interest is focused is a separate set of several parameters crucial to the model, and in the case of calibration of successive versions of a modified model — parameters usually connected with terms newly introduced into the equations. When comparing the obtained values assumed by the state variables in a model and the real system, the author of a model tries to adjust the values of unknown parameters. In a situation where this approach does not give

positive results, the values, of other parameters present in the model are modified. The application of this method has the advantage that it makes possible to assess the results from simulation on the basis of not only an available set of measurement data, but also on the basis of the author's experience and theoretical knowledge. Moreover, the use of a subjective criterion permits the author to take into account model-adjustment quality criteria, difficult to formalize, such as the time of occurrence of the maximum values, the size of these values, change amplitude, the mean value and such like.

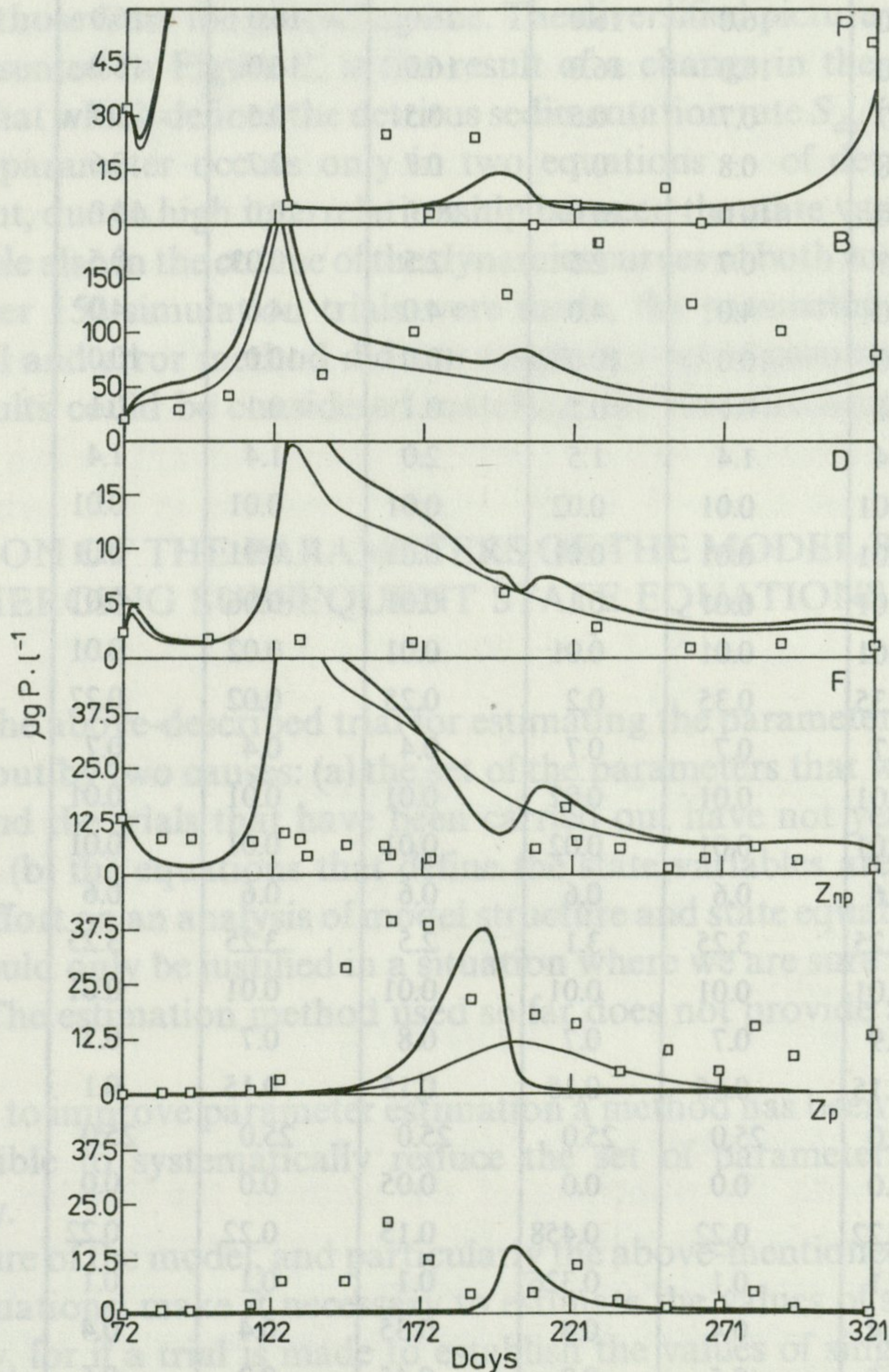


Fig. 2. A comparison of the solutions of the model with measurement data. Solid thinner line — results from simulation for parameter version 15 (see Table 4), thicker solid line — results from simulation for parameter version 16, squares — measurement data, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — concentration of inorganic phosphorus

Table 4. Parameter values of some versions of the model

Parameter	Model version number							
	15	16	406	513	615	22	21	326
P_1	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6
P_2	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
P_3	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
I_{opt}	1464.4	1464.4	1464.4	1464.4	1464.4	1464.4	1464.4	1464.4
T_f^{opt}	16.0	16.0	16.0	16.0	16.0	16.0	16.0	16.0
T_b^{opt}	16.0	16.0	16.0	16.0	16.0	16.0	16.0	16.0
g_2	0.7	0.7	0.5	0.5	0.5	0.7	0.7	0.25
g_1	0.8	0.8	0.7	0.7	0.7	0.6	0.6	0.1
K_d	10.0	10.0	20.0	20.0	20.0	10.0	12.0	20.0
G_f^{max}	0.7	0.7	2.5	2.5	0.03	0.5	0.6	0.7
K_{max}	4.0	4.0	4.0	4.0	4.0	4.0	4.0	4.0
G_b	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
C_d	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
G_{znp}^{max}	1.4	1.4	1.5	2.0	1.4	1.4	1.4	5.0
K_n^2	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
m_b	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
m_{znp}	0.01	0.01	0.1	0.01	0.06	0.01	0.01	0.06
m_{zp}	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.02
m_f	0.35	0.35	0.2	0.25	0.02	0.27	0.27	0.25
A_{zn}	0.7	0.7	0.7	0.4	0.4	0.7	0.7	0.4
K_n^1	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
K_n^3	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
A_{zp}	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6
G_{zp}^{max}	3.25	3.25	3.1	2.5	3.25	3.25	3.25	4.5
K_p	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
S_{det}	0.9	0.7	0.7	0.8	0.7	0.7	0.7	0.7
m	0.15	0.15	0.15	0.15	0.15	0.1	0.17	0.15
T_z^{opt}	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0
S_p	0.0	0.0	0.0	0.05	0.0	0.0	0.0	0.0
q_{znp}	0.22	0.22	0.458	0.15	0.22	0.22	0.22	0.22
q_{zp}	0.1	0.1	0.326	0.1	0.1	0.1	0.1	0.1
C_2	0.4	0.4	0.4	0.35	0.4	0.4	0.4	0.35
C_1	0.5	0.5	0.2	0.45	0.2	0.5	0.5	0.45

Due to the presence, in the model considered, of several dozen parameters it was impossible to try to use any formal algorithms, and it was necessary to use the trial and error method, particularly because information was available about the value ranges of some parameters.

In accordance with the principles of the trial and error method, excluded from the estimation were all those parameters whose values had been measured in the environment, as well as those whose values ecologists had estimated on the basis of earlier experiments. All other parameters of the model were subjected to estimation.

Parameter estimation by the trial and error method proved to be very difficult primarily because the set of parameters of unknown values was still very numerous. Besides, due to the interrelationships between the state equations, through variables and parameters, the possibility to control the response of the model to a value change of even a single parameter was small, and the results from each next simulation were often far worse than those from the preceding one. The diversified picture of the responses of the model, presented in Figure 2, is the result of a change in the value of only one parameter — that which defines the detritus sedimentation rate S_{det} (versions 15 and 16 Table 4). The parameter occurs only in two equations — of detritus and bacteria dynamics — but, due to high interrelationship between the state variables, a change in its value is visible also in the course of the dynamics curves of both zooplankton groups.

Though over 150 simulation trials were made, the parameter estimation by the traditional trial and error method did not result in a set of parameters for which the simulation results could be considered matching the measurements.

4. ESTIMATION OF THE PARAMETERS OF THE MODEL BY THE STEP BY STEP MERGING SUBSEQUENT STATE EQUATIONS METHOD

Failure of the above-described trial for estimating the parameters of the model can be brought about by two causes: (a) the set of the parameters that were estimated was still too big, and the trials that have been carried out have not yet determined their correct values, (b) the equations that define the state variables are wrong.

Focusing effort on an analysis of model structure and state equations to prove their correctness would only be justified in a situation where we are sure we are not dealing with case (a). The estimation method used so far does not provide a good ground for that.

In an effort to improve parameter estimation a method has been worked out which makes it possible to systematically reduce the set of parameters to be estimated simultaneously.

The structure of the model, and particularly the above-mentioned interrelationship between its equations, make it necessary to estimate the values of several parameters simultaneously, for if a trial is made to establish the values of single parameters, the remaining, still not estimated parameters often have a definitely greater effect on the simulation results, and make it impossible to obtain a correct estimated value.

It has been suggested that the need to eliminate the adverse effect of the parameters present in the model equations should be met by replacing the solution of some of the state equations with the values of the state variables defined by them. For this reason, it was decided to supplement the model with approximations of the state-variable values,

obtained from available measurement data. The reduction, brought about by that, of the number of state equations to be evaluated and of the parameters estimated simultaneously allows for a better control and more efficient parameter estimation by the traditional method. If measurements provided sufficient information on the real dynamics of the phenomena occurring in an ecosystem, and the approximated changes, determined from them, of the state variables were a sufficiently exact picture of the behaviour of a system, one might expect the parameter values established by estimation, leaving out some variables, to be also true after the addition of the state equations eliminated initially.

Since the modelling practice indicates that the author of a model does not usually dispose of a good set of measurement data, and a mathematical model is the description of a very much reduced system in comparison to a real ecosystem, the assumptions concerning the application of the proposed method are seldom satisfied. It may be expected, however, that the method described in this paper will provide good initial approximations of the parameters to be estimated, with a relatively small number of simulations.

The proposed method of step by step merging subsequent state equations (*SMSSE*) can only be used when suitable approximations have been found for the variation of all state variables on the basis of existing measured values. Advantage can be taken of the rule that a time series x_i , $i = 1, 2, \dots, N$ can be presented in the form of a discrete expansion in a Fourier series:

$$x_i = A_0 + \sum_{j=1}^S [A_j \cdot \cos(j2\pi/N) + B_j \cdot \sin(j2\pi/N)]$$

$$A_j = 2/N \sum_{i=1}^N x_i \cos(j2\pi_i/N)$$

$$B_j = 2/N \sum_{i=1}^N x_i \sin(j2\pi_i/N)$$

$$A_0 = 1/N \sum_{i=1}^N x_i$$

where S — number of harmonics in a Fourier expansion.

In accordance with the principles of the method, the number of parameters estimated simultaneously was reduced and simulation results were examined for a model which initially consisted of only two differential equations, whereas the values of other state variables were given in the form of Fourier series approximating the measurements. The modelled state variables were the concentration of phosphorus and of predatory zooplankton, due to which the number of parameters to be estimated was reduced to 6. Since most of the processes occurring in natural ecosystems are characterized by seasonality and oscillations related to an annual cycle, Fourier-series approximation was used with a 360-day basic period.

Such an initial system of state equations and approximations seems useful for several reasons. Predatory zooplankton is the last link of the food chain of the

ecosystem modelled (planktivorous fish were not taken into account in the model), so it regulates the lower trophic levels. Phosphorus pool provides the basic source of this nutrient for the producers and reducers represented in the model by the phytoplankton and bacteria, respectively. It may, therefore, be assumed that both the state variables modelled are quantities of principal importance for the dynamics of the processes taking place in the system. Figure 3 represents this stage of parameter estimation (version 406 parameters have been summarized in Table 4).

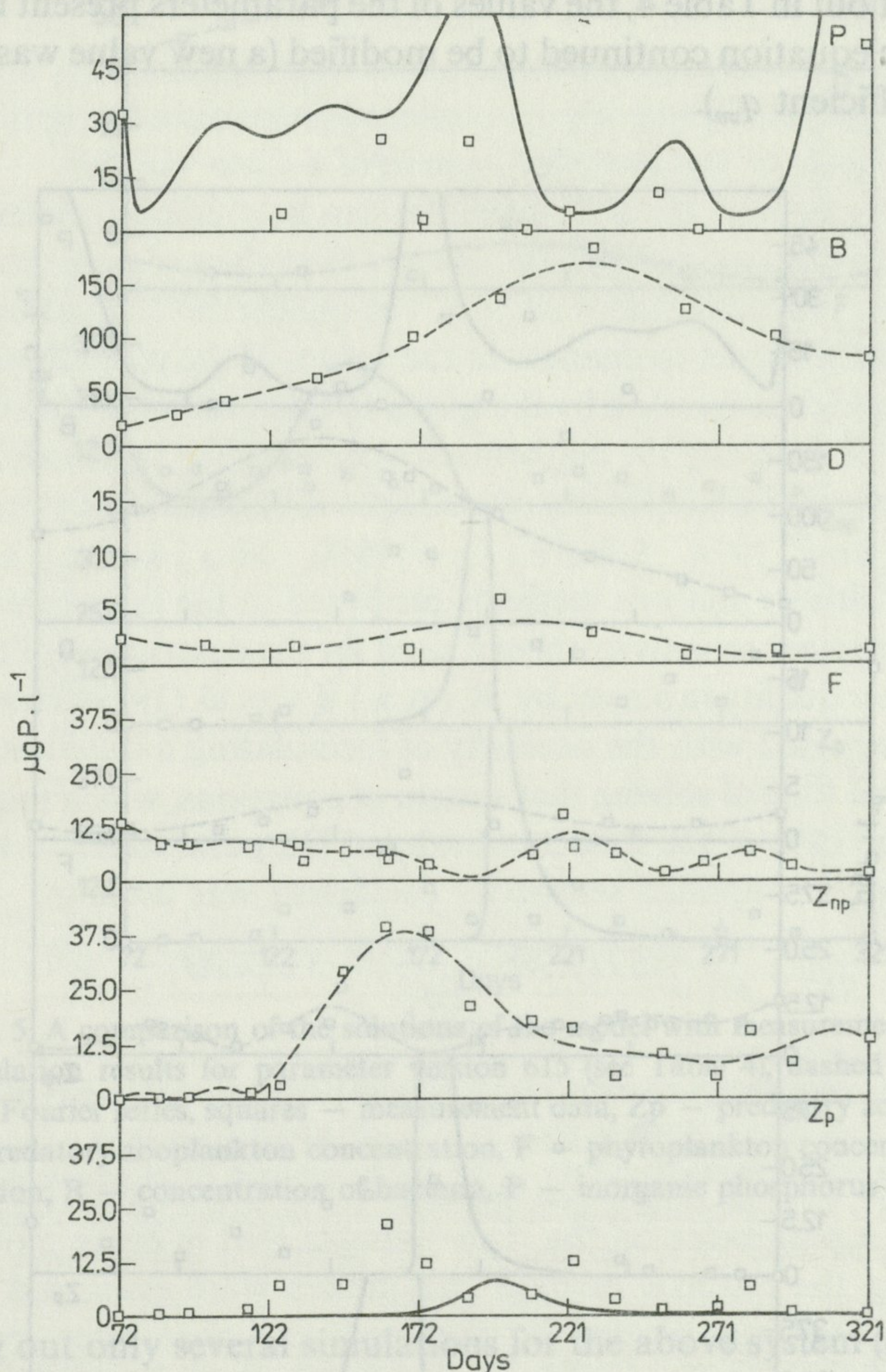


Fig. 3. A comparison of the solutions of the model with measurement data. Solid line — simulation results for parameter version 406 (see Table 4), dashed line — measurement approximation by Fourier series, squares — measurement data, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — concentration of inorganic phosphorus.

In a particular configuration of differential equations and approximating formulas calibration of the model was only continued up to the moment when state-variable values were obtained which permitted a further equation to be added to replace the

corresponding approximation expression. Parameter set no. 406, for which simulation results have been presented in Figure 3, was considered appropriate for adding the third differential equation.

It is useful to merge equations in the order of their defining the dynamics of lower and lower food levels. The third to be introduced into the system was the nonpredatory zooplankton state equation. In the estimation of that system it proved necessary to correct the values of the parameters estimated at the preceding stage. As indicated by the parameters set out in Table 4, the values of the parameters present in the predatory zooplankton state equation continued to be modified (a new value was determined for the excretion coefficient q_{zn}).

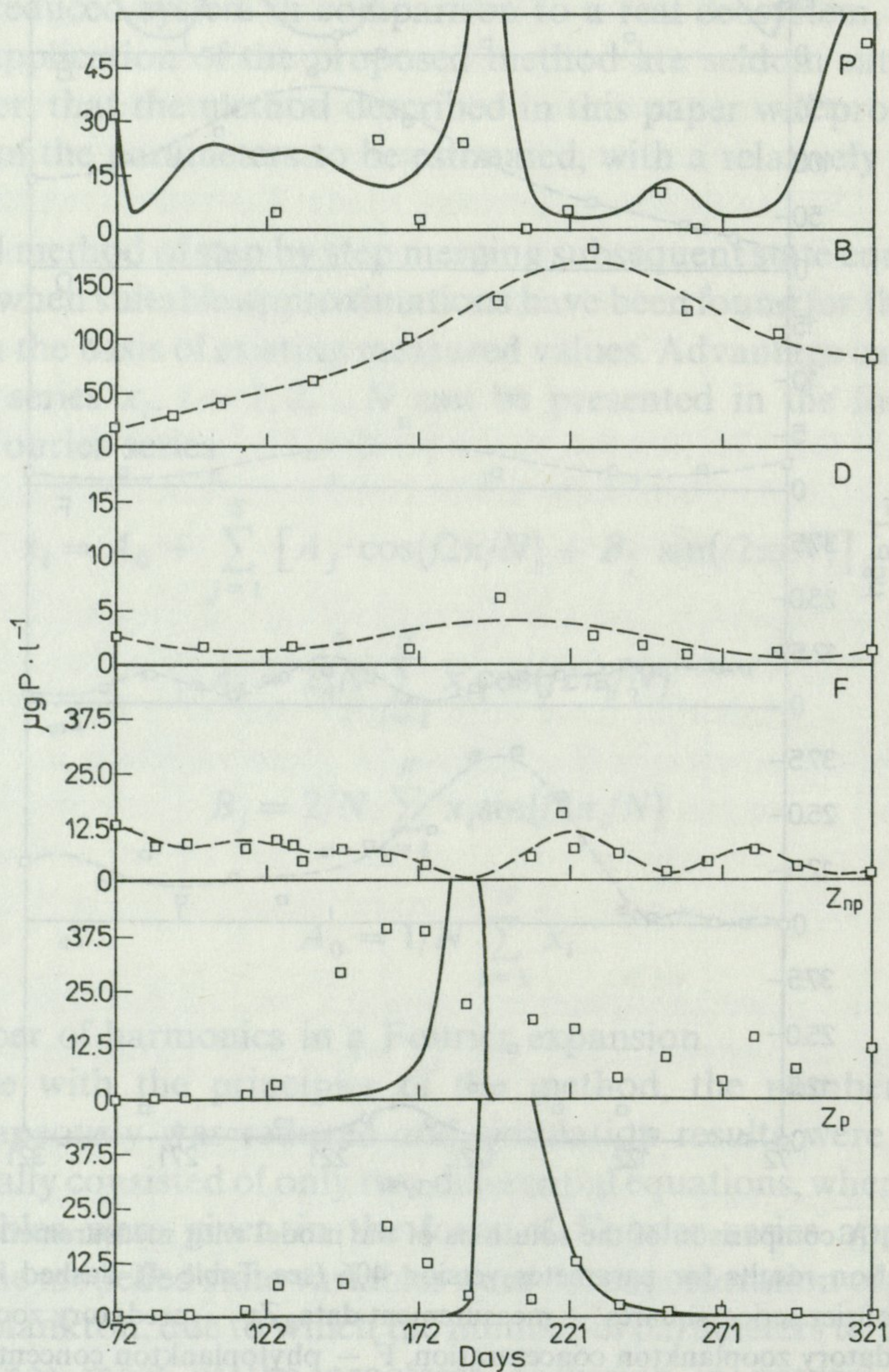


Fig. 4. A comparison of the solutions of the model with measurement data

Solid line — simulation results for parameter version 513 (see Table 4), dashed line — measurement approximation by Fourier series, squares — measurement data, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — concentration of inorganic phosphorus

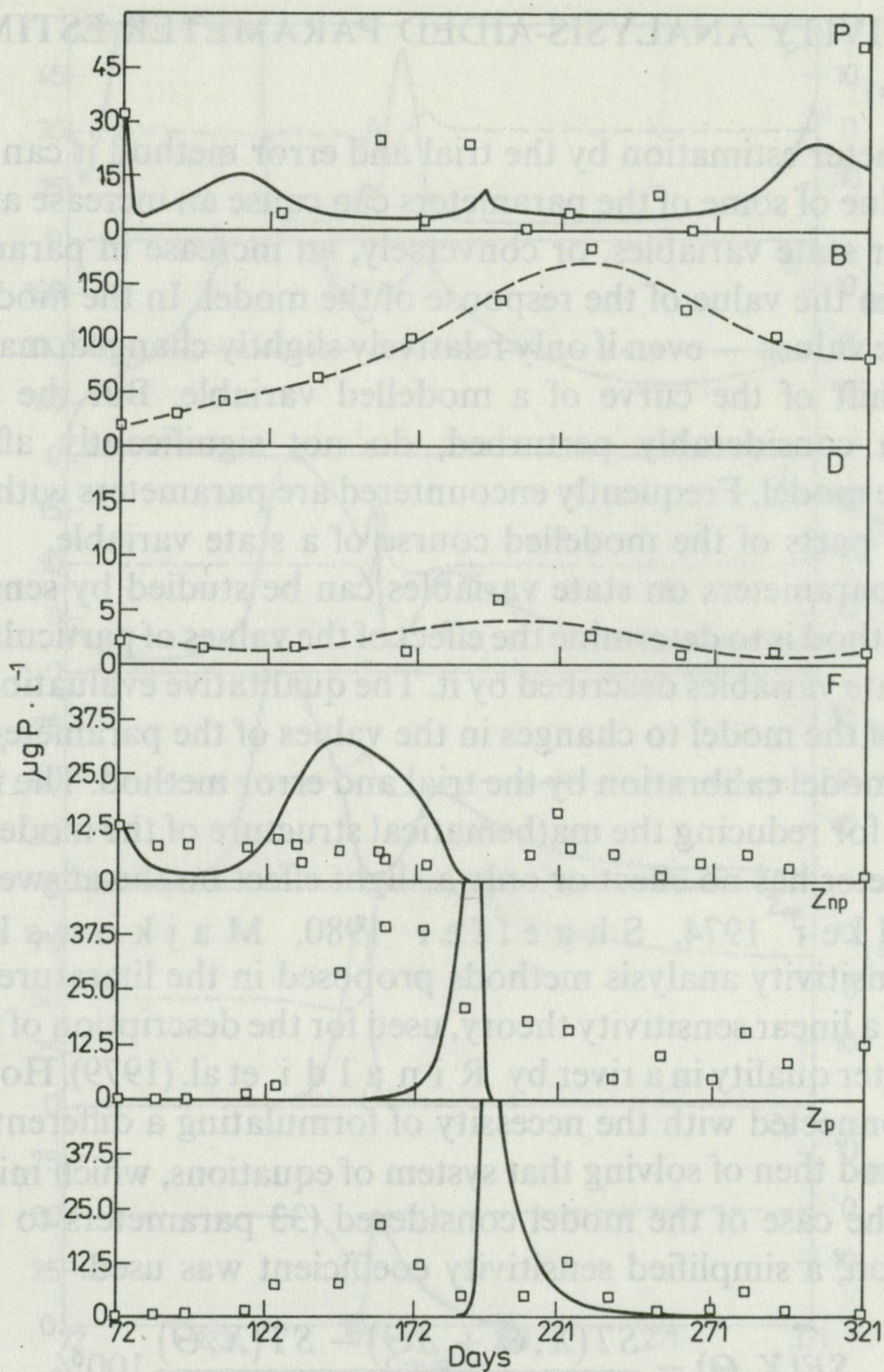


Fig. 5. A comparison of the solutions of the model with measurement data

Solid line — simulation results for parameter version 615 (see Table 4), dashed line — measurement approximation by Fourier series, squares — measurement data, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — inorganic phosphorus concentration

By carrying out only several simulations for the above system (e.g. version 513 in Figure 4) parameter estimates were obtained which made it possible to replace a further approximating series with an equation for the phytoplankton. Simulation results for a parameter version (version 615 Table 4) have been presented in Figure 5.

Following the introduction of the fifth state equation, defining changes in the concentration of bacteria, the carrying out of several simulations made it possible to add the last differential equation, eliminated so far.

5. SENSITIVITY ANALYSIS-AIDED PARAMETER ESTIMATION

During parameter estimation by the trial and error method it can be seen that an increase in the value of some of the parameters can cause an increase also in the values obtained by other state variables, or conversely, an increase in parameter value can cause a decrease in the value of the response of the model. In the model there may be parameters whose values — even if only relatively slightly changed, may correspond to a considerable shift of the curve of a modelled variable. But the values of other parameters, even considerably perturbed, do not significantly affect the results obtained from the model. Frequently encountered are parameters with a varying effect on the particular parts of the modelled course of a state variable.

The effect of parameters on state variables can be studied by sensitivity analysis. The aim of the method is to determine the effect of the values of particular parameters of a model on the state variables described by it. The qualitative evaluation thus obtained, on the response of the model to changes in the values of the parameters estimated can be very useful in model calibration by the trial and error method. The method can also provide the basis for reducing the mathematical structure of the model, proving that a particular parameter has no effect or only a slight effect on the answer obtained from the model (Miller 1974, Shaeffer 1980, Majkowski et al. 1981).

One of the sensitivity analysis methods proposed in the literature is an analytical method based on a linear sensitivity theory, used for the description of the properties of a model of the water quality in a river by Rinaldi et al. (1979). However, the use of this method is connected with the necessity of formulating a differential equation for each parameter, and then of solving that system of equations, which might prove a very difficult task in the case of the model considered (33 parameters to be estimated).

For this reason, a simplified sensitivity coefficient was used:

$$SE(X, \Theta) = \frac{ST(X, \bar{\Theta} + \Delta\Theta) - ST(X, \bar{\Theta})}{ST(X, \bar{\Theta})} 100\%$$

where: $SE(X, \Theta)$ — sensitivity coefficient, $ST(X, \bar{\Theta})$ — nominal value of a state variable, $ST(X, \bar{\Theta} + \Delta\Theta)$ — state-variable value at a perturbed nominal parameter value.

This coefficient usually illustrates the effect of a one-percent perturbation in the nominal value of a parameter on the state variable that is being modelled.

Then by using the *SMSSE* method parameters were estimated and sensitivity curves were calculated and plotted for the successive parameters present in newly added state equations. On their basis the direction was inferred of the influence of parameter value changes on the value and form of the responses of the model. In subsequent simulations parameter values were modified according to the expected effect on the course of the variables being modelled. This made it possible to find the values primarily of those parameters which had the greatest effect on the simulation results.

In Figure 6 an example has been presented of sensitivity curves for a set of 6 state equations. Table 4 contains those parameters of the model which correspond to that

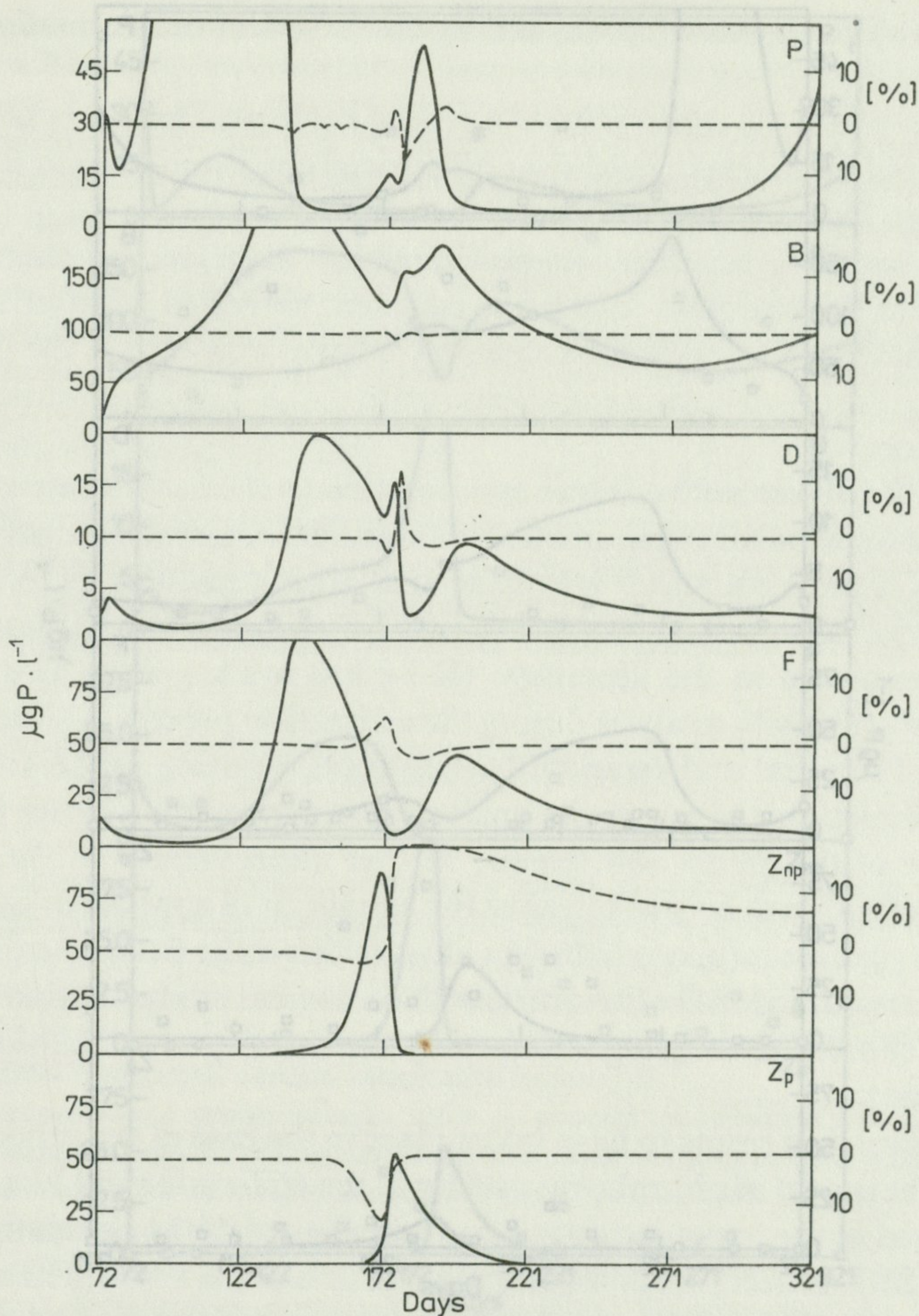


Fig. 6. A comparison of the solution of the model with measurement data

Solid line — simulation result for parameter version 22 (see Table 4), dashed line — curve of the sensitivity coefficient representing a percent-change in the value of state variable, caused by a one-percent change in parameter m in comparison to its nominal value, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — concentration of inorganic phosphorus

version (22). An analysis of the curves shows that a one-percent perturbation in the value of parameter m present only in the equation defining the concentration of bacteria does not affect the value of this variable, yet it affects other quantities that are being modelled. Particularly important is its effect on the curve for nonpredatory and predatory zooplankton.

Version 21, presented in Figure 7, was obtained when all conclusions from the above sensitivity analysis of selected parameters, used in connection with the *SMSSE* method, were taken into account. In comparison to version 22 (see Figure 6), curves for the concentration of bacteria and both zooplankton groups were far closer to their

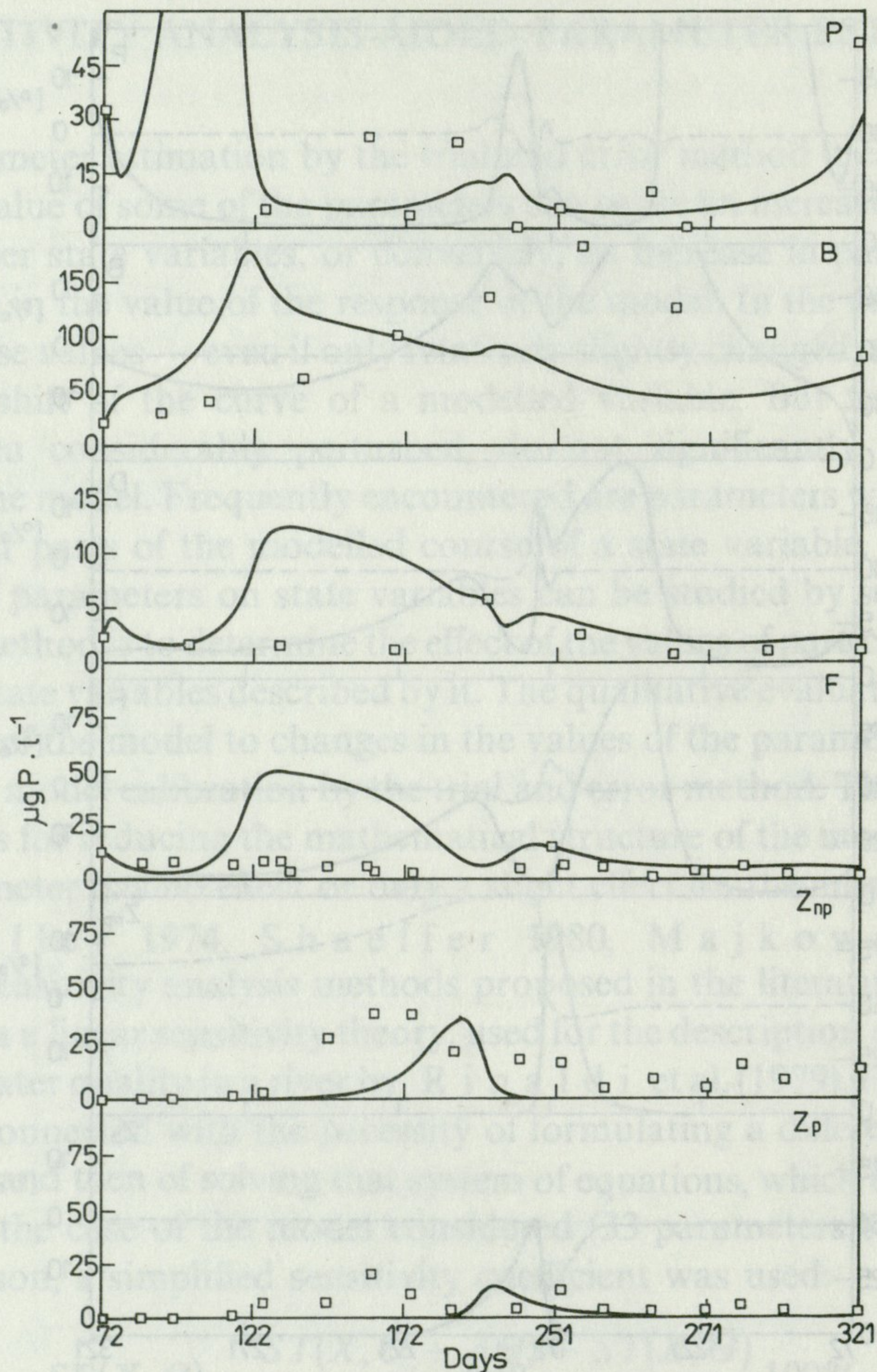


Fig. 7. A comparison of the solutions of the model with measurement data

Solid line — simulation results for parameter version 21 (see Table 4), squares — measurement data, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — concentration of inorganic phosphorus

measured values. The results seem better than the previous ones, although still far from agreeing with measurement data.

Figure 8 presents the response of the model for version 326 obtained from parameter estimation by the step by step merging subsequent state equations method combined with sensitivity analysis. An analysis of the sensitivity, made for this version, of the equations of the model to all the parameters present in it has shown that in the case of over 20 parameters the sensitivity coefficient curves attain values exceeding 20%.

To close with it may be worthwhile to stress the fact that plotted for various versions of the model, curves of sensitivity to the same parameter can definitely differ.

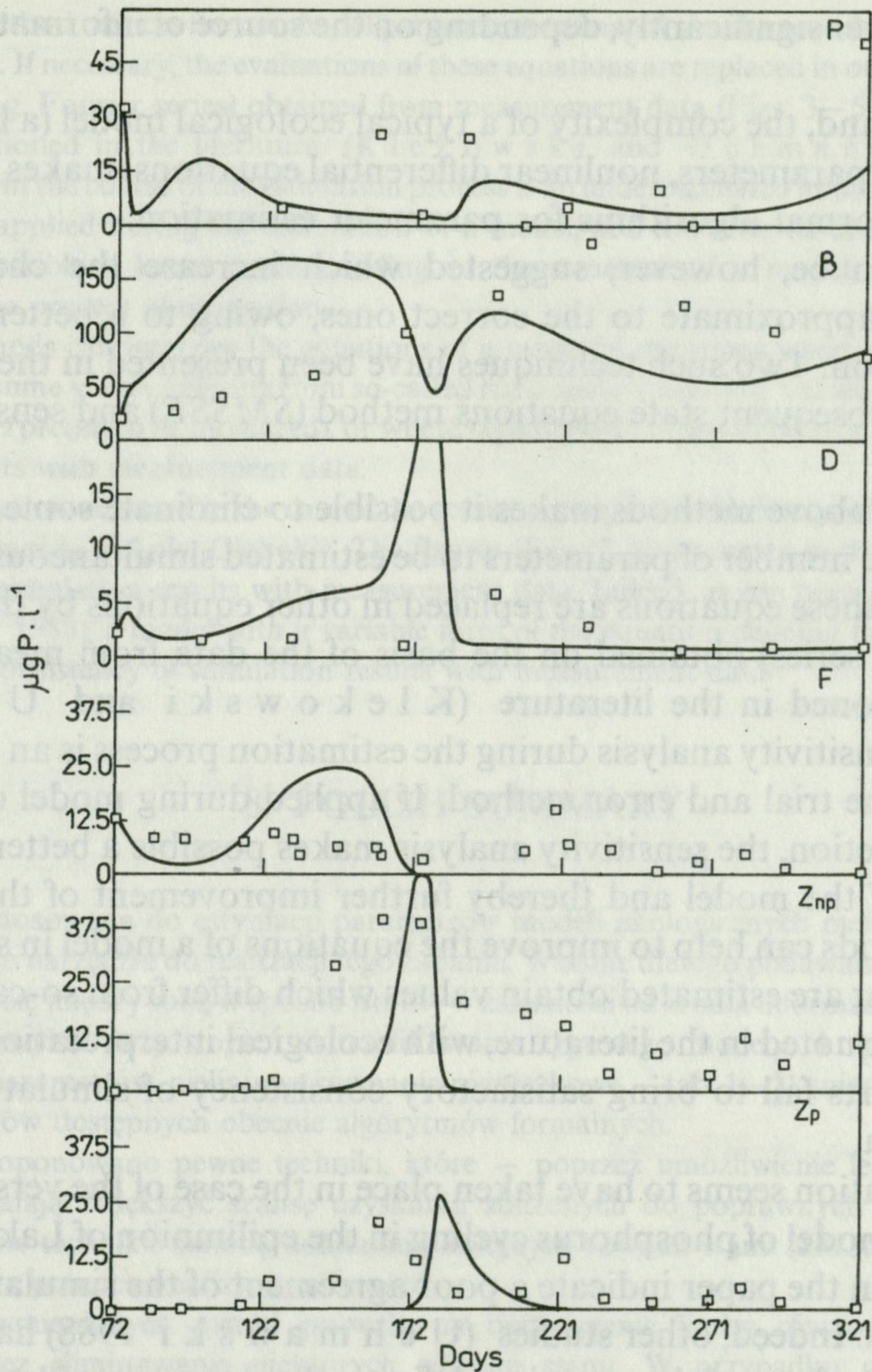


Fig. 8. A comparison of the solutions of the model with measurement data

Solid line — simulation results for parameter version 326 (see Table 4), squares — measurement data, Z_p — predatory zooplankton concentration, Z_{np} — nonpredatory zooplankton concentration, F — phytoplankton concentration, D — detritus concentration, B — concentration of bacteria, P — inorganic phosphorus concentration

Conclusions concerning the sensitivity of a model to the parameters that are being estimated are binding only in the case of small deviations from the nominal value.

6. CONCLUSIONS

The author's experience (Loga 1984) and that of other authors (Fedra et al. 1980) indicate that the traditional method of trials and errors commonly used for the estimation of the parameters of ecological models is not an efficacious tool if used to perform this task. It is for this reason that the parameter values given in the literature

differ from each other significantly, depending on the source of information from which they come.

On the other hand, the complexity of a typical ecological model (a large number of state variables and parameters, nonlinear differential equations) makes it impossible to use the available formal algorithms for parameter estimation.

Techniques can be, however, suggested which increase the chance to obtain parameter values approximate to the correct ones, owing to a better control of the process of estimation. Two such techniques have been presented in the paper: the step by step merging subsequent state equations method (*SMSSE*) and sensitivity analysis-aided estimation.

The first of the above methods makes it possible to eliminate some state equations and thus reduce the number of parameters to be estimated simultaneously. If necessary, the evaluations of these equations are replaced in other equations by their approximations (e.g. Fourier series) obtained on the basis of the data from measurements.

Though mentioned in the literature (K l e k o w s k i and U c h m a ń s k i 1980), the use of sensitivity analysis during the estimation process is an underestimated improvement of the trial and error method. If applied during model calibration, and not after its completion, the sensitivity analysis makes possible a better understanding of the structure of the model and thereby further improvement of the estimation.

Both the methods can help to improve the equations of a model in situations where the parameters that are estimated obtain values which differ from so-called reasonable values (e.g. values quoted in the literature, with ecological interpretation or measured), or if repeated efforts fail to bring satisfactory consistency of simulation results with measurement data.

The latter situation seems to have taken place in the case of the version, analysed in this paper, of the model of phosphorus cycling in the epilimnion of Lake Głębokie. The figures presented in the paper indicate a poor agreement of the simulation results with measurement data. Indeed, other studies (U c h m a ń s k i 1988) have shown that a model with another form of the equation defining the dynamics of bacteria gives a far better consistency of simulation results with measurements. In the model version here considered the bacteria took up phosphorus and were the intermediate link in detritus mineralization. In a later version the bacteria take up detritus and release phosphorus.

7. SUMMARY

The trial and error method widely used for the estimation of the parameters of ecological models is not an efficient tool if used to perform this task. For this reason, parameter values quoted in the literature differ from one another significantly, depending on the source of information from which they come.

The complexity, usually high, of a typical ecological model (a large number of state variables and parameters, nonlinear differential equations — Tables 1 — 3) makes it impossible to use formal algorithms, now available, for the estimation of parameters.

In the paper certain techniques have been suggested which can increase the chance to obtain parameter values approximate to the correct ones through a better control of the process of estimation. Two such techniques have been presented: the step by step merging subsequent state equations method (*SMSSE*) and sensitivity analysis-aided estimation.

The former method reduces the number of parameters estimated simultaneously, by eliminating some of the state equations. If necessary, the evaluations of these equations are replaced in other equations with their approximations (e.g. Fourier series) obtained from measurement data (Figs. 3–5).

Though mentioned in the literature (K l e k o w s k i and U c h m a ń s k i 1980), the use of sensitivity analysis in the course of the estimation process is an underestimated improvement of the trials and errors method. If applied during the calibration of a model, and not after its completion, the sensitivity analysis makes possible a better understanding of the structure of a model, and thereby a further improvement of the process of estimation.

Both the methods can improve the equations of a model in situations where the parameters that are being estimated assume values differing from so-called reasonable values (e.g. values quoted in the literature, with ecological interpretation or measured), or where repeated efforts fail to bring a satisfactory consistency of simulation results with measurement data.

The latter situation occurred in the case of the version, analysed in this study, of a model of phosphorus cycling in the epilimnion of Lake Głębokie. The figures (Figs. 7, 8) presented in the paper indicate a poor consistency of the simulation results with measurement data. Indeed, as has been shown by other studies (U c h m a ń s k i 1988), a model with a variable form of the equation defining the dynamics of bacteria gives a far better consistency of simulation results with measurement data.

8. POLISH SUMMARY

Powszechnie stosowana do estymacji parametrów modeli ekologicznych metoda prób i błędów nie stanowi skutecznego narzędzia do realizacji tego zadania. Właśnie dlatego podawane w literaturze wartości parametrów różnią się między sobą w sposób istotny w zależności od źródła informacji, z którego pochodzą.

Występujący zwykle duży stopień skomplikowania typowego modelu ekologicznego (duża liczba zmiennych stanu i parametrów, nieliniowe równania różniczkowe — tab. 1–3) uniemożliwia stosowanie do estymacji parametrów dostępnych obecnie algorytmów formalnych.

W pracy zaproponowano pewne techniki, które — poprzez umożliwienie lepszej kontroli procesu estymacji — pozwalają zwiększyć szansę uzyskania zbliżonych do poprawnych wartości parametrów. Pokazano dwie takie techniki: metodę dołączania kolejnych równań stanu (SMSSE) oraz wspomaganie procesu estymacji za pomocą analizy wrażliwości.

Pierwsza z wymienionych metod pozwala na ograniczenie liczby równocześnie estymowanych parametrów poprzez eliminowanie niektórych równań stanu. W przypadku gdy jest to konieczne rozwiązania tych równań są zastępowane w pozostałych równaniach przez ich aproksymaty (np. szeregi Fouriera) otrzymywane na podstawie danych pomiarowych (rys. 3–5).

Stosowanie analizy wrażliwości w toku procesu estymacji, jakkolwiek sygnalizowane w literaturze (K l e k o w s k i i U c h m a ń s k i 1980) jest niedocenianym usprawnieniem metody prób i błędów. Przeprowadzenie analizy wrażliwości podczas kalibracji modelu, a nie dopiero po jego zakończeniu, pozwala na lepsze zrozumienie struktury modelu i przez to dalsze usprawnienie procesu estymacji.

Obie te metody mogą doprowadzić do poprawienia równań modelu, w przypadku gdy estymowane parametry przybierają wartości odbiegające od tzw. rozsądnych wartości (np. wartości podawanych w literaturze, posiadających interpretację ekologiczną lub zmierzonych), albo gdy mimo wielokrotnych wysiłków nie udaje się uzyskać zadowalającej zgodności wyników symulacji z danymi pomiarowymi.

Ta ostatnia sytuacja zaistniała w przypadku analizowanej w tej pracy wersji modelu krążenia fosforu w epilimnionie Jeziora Głębokiego. Przedstawione rysunki (rys. 7, 8) wskazują na nienajlepszą zgodność wyników symulacji z pomiarami. I rzeczywiście inne prace pokazały (U c h m a ń s k i 1988), że model ze zmienioną postacią równania opisującego dynamikę bakterii daje znacznie lepszą zgodność wyników symulacji z pomiarami.

9. REFERENCES

1. Benson M. 1979 — Parameter fitting in dynamics models — *Ecol. Model.* 6: 97—115.
2. Fedra K., van Straten G., Beck M. B. 1980 — Uncertainty and arbitrariness in ecosystem modelling: a lake modelling example — IIASA, Laxenburg, Austria, WP-80-87.
3. Jørgensen S. E., Jørgensen L. A., Kamp-Nielsen L., Mejer M. F. 1981 — Parameter estimation in eutrophication modelling — *Ecol. Model.* 13: 11—129.
4. Klekowski R. Z., Uchmański J. 1980 — Sensitivity analysis of energy flow model by Monte Carlo method — *Pol. ecol. Stud.* 6: 55—59.
5. Kraszewski A. K. 1982 — Metody poprawy własności eksploatacyjnych modeli jakości wody w rzece [Methods of improvement of some usage characteristics of water quality models] — Ph.D. Thesis, Warsaw Technical University, Warsaw, 133 pp.
6. Lewis S., Nir A. 1978 — A study of parameter estimation procedures of a model of lake phosphorus dynamics — *Ecol. Model.* 4: 99—117.
7. Loga M. 1984 — Analiza możliwości usprawnienia procesu estymacji parametrów modelu obiegu fosforu w ekosystemie jeziora [The analysis of the possibility of improvement of parameter estimation in phosphorus cycle model of the lake ecosystem] — M.Sc. Thesis, Warsaw Technical University, Warsaw, 147 pp.
8. Majkowski J., Ridgeway J. M., Miller D. R. 1981 — Multiplicative sensitivity analysis and its role in development of simulation models — *Ecol. Model.* 12: 191—208.
9. Miller D. R. 1974 — Sensitivity analysis and validation of simulation models — *J. theor. Biol.* 48: 345—360.
10. Rinaldi S., Soncini-Sessa R., Sthefest M., Tamura M. 1979 — Modelling and control of river quality — McGraw-Hill, New York, 380 pp.
11. Shaefter D. L. 1980 — A model evaluation methodology applicable to environmental assessment models — *Ecol. Model.* 8: 275—298.
12. Uchmański J. 1988 — Simulation model of phosphorus cycling in the epilimnion of Lake Głębokie — *Ekol. pol.* 36: 347—386.

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