

MODELLING THE DISSOLVED OXYGEN
CHANGE IN STREAMS USING
NONLINEAR REGRESSION ANALYSIS

by

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MANAGEMENT PERSPECTIVE

Several indirect methods are presented for simultaneously estimating the component rates for production, diffusion and respiration from evenly spaced (hourly) measurements of dissolved oxygen at a single river station. The procedures allow us to evaluate the adequacy of dissolved oxygen models and particularly the photosynthesis-light relationship. Furthermore, an approach is also given for providing confidence intervals for the estimates of each component. The findings of this paper permit comparing the productivity in different streams or at different stations within the stream, and to evaluate change over time.

PERSPECTIVE ADMINISTRATIVE

Ce rapport présente plusieurs méthodes indirectes qui permettent d'estimer simultanément les vitesses de production, de diffusion et de respiration à partir de mesures espacées (intervalles d'une heure) de l'oxygène dissous à une station unique en rivière. Ces procédures nous permettent d'évaluer l'exactitude des modèles de l'oxygène dissous et, notamment, le rapport photosynthèse-lumière. Une méthode est également donnée pour déterminer des intervalles de confiance pour l'estimation de chaque composante. Les résultats de cette étude permettent de comparer la productivité dans différents cours d'eau ou à différentes stations situées sur le même cours d'eau et d'évaluer les changements dans le temps.

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SUMMARY

The application of nonlinear regression analysis to observed stream dissolved oxygen concentrations, by means of an oxygen mass-balance equation, provided estimates of the model parameters, which enabled further determination of the component processes in the oxygen metabolism in a segment of flowing water. The procedure was also used to identify photosynthesis-light (P-I) models for a Canadian river.

Five P-I models were examined and, although none of the models was accepted as strictly adequate, the study showed that the goodness of fit was substantially improved by using nonlinear photosaturation and photoinhibition models. No distinct photoinhibition was observed

within the range of light intensity that occurred during the data period. Moreover, since none of the nonlinear models showed a significantly better fit to the data, we may conclude that any of the equations (4), (6) or (8) can be used for assessing the component rates of dissolved oxygen change.

INTRODUCTION

Four main processes affect the concentration of dissolved oxygen in a natural stream. They are: photosynthetic production, diffusion, respiration and drainage accrual. There is a release of oxygen into the water as a result of photosynthetic primary production. Diffusion is an exchange of oxygen with the air in a direction depending on the saturation gradient. There is an uptake of oxygen from the water as a result of the respiration of benthic or planktonic organisms and chemical oxidation. There may also be an influx of oxygen with accrual of ground water and surface drainage. All these factors interact to produce the daily curve of oxygen change in a segment of flowing water. These processes may be quantitatively summarized as follows:

$$q = p + d - r + a \quad (1)$$

where q , p , d , r and a are expressed in concentration units (i.e., $\text{g m}^{-3} \text{h}^{-1}$) and denote the rates of change of dissolved oxygen, primary

production, diffusion, respiration and drainage accrual, respectively (Odum, 1956). In the present study, accrual is assumed to be negligible relative to the other influences. Respiration is assumed to be constant (Odum, 1956; Schurr and Ruchti, 1975). We wish to propose here simple indirect methods for determining simultaneously the component rates of production, diffusion and respiration from the analysis of the observed curve of dissolved oxygen assuming the data record consists of systematically one hour-spaced measurements from a single station. The procedure is based on regression analysis applied to nonlinear models which are derived from equation (1). It is further assumed that the stream studied is homogeneous, in the sense that the rates of photosynthesis, diffusion and respiration are the same in all sections of the river.

A variety of methods have been used to evaluate the different components of equation (1). Some of these methods (e.g., the method pioneered by Odum, 1956) suffer from a lack of mathematical closeness and may therefore give very approximate results. Other procedures have been developed on the basis of very stringent hypotheses; for example, in the models developed by Schurr and Ruchti (1975), the authors assumed proportionality between production and light intensity though such an assumption may be valid for low light intensities only (Cosby and Horberger, 1984).

It is the specific purpose of this work to present mathematical expressions that incorporate the effects of light intensity and

temperature of the water and to demonstrate their application in the analysis of the temporal distribution of dissolved oxygen observed in Canagagigue Creek (Ontario). It is well known that temperature influences the rates of the physical and biochemical reactions that affect dissolved oxygen concentration, and also the rate and the direction of exchange of oxygen with the air through the oxygen saturation concentration of the water, which is a function of temperature and the atmospheric pressure (Hutchinson, 1957). Photosynthesis in relation to light intensity is a major topic in the study of primary productivity of water. The understanding and calculation of primary production is assisted by mathematical formulations of the photosynthesis-light relationship which contain biologically significant parameters. The photosynthesis-light relationship can be generalized as follows: photosynthesis increases linearly with light at low light intensities, becomes approximately constant at higher intensities (photosaturation) and in some cases begins to decline at even higher intensities (photoinhibition) (Cosby and Hornberger, 1984). Many mathematical models for describing this curvilinear relationship have been reported in the literature and a comparison of the fit of several models with the photosynthesis-light curves of natural phytoplankton populations has been performed by Iwakuma and Yasuno (1983) and Cosby et al. (1984).

THE MODELS

The models presented in this section differ mainly in the formulation of the productivity-light relation while the diffusion rate has always been assumed to be proportional to the difference (Δy) between the real dissolved oxygen concentration (y) in the water and its saturation value (O_s) (i.e., $\Delta y = O_s - y$). If we except the first model considered below, the equations used lead to nonlinear models and a method is given for assessing the parameters related to the various component rates. Although the algorithm used for estimating these parameters follows the same general scheme for all the models, a detailed description of the procedure will be developed for each case.

The general expression for the model is

$$q = f(I) + k \Delta y - r + e \quad (2)$$

where q is the $n \times 1$ vector of observations (i.e., $q_t = y_{t+1} - y_t$, that is the difference of two successive values of the observed dissolved oxygen) f is a function of the light intensity I ($E m^{-2} h^{-1}$) measured for $t = 1, \dots, m$, k is the reaeration coefficient (h^{-1}) and e is the $n \times 1$ vector of which the n elements are assumed to be independent normal variables each with zero mean and variance σ^2 .

• Model 1

If f is assumed to be a linear function of I , equation (2) becomes

$$q = \alpha I + k \Delta y - r + e \quad (3)$$

and the parameters α , k and r can then be estimated directly by using linear regression analysis.

• Model 2

The second model we considered, which is a photoinhibition model, is obtained by replacing $f(I)$ in equation (2) by Steele's formula (Steele, 1962) as an equation for describing photosynthesis-light curve (i.e., $f(I) = P_{\max} (I/I_s)(e^{1-I/I_s})$). This equation has two parameters: a maximum rate of photosynthesis (P_{\max}) and the light intensity (I_s) at which the initial slope line reaches P_{\max} before it decreases (photoinhibition effect).

Hence, the expression of q is given as

$$q = \alpha I e^{1-\beta I} + k \Delta y - r + e \quad (4)$$

where $\alpha = P_{\max}/I_s$ and $\beta = 1/I_s$.

Estimation of the parameters of the model

Since the right hand side of regression equation (4) is not linear in all of the parameters, estimation of α , β , k and r will require an iterative procedure which can be described as follows:

- (i) Using first-order Taylor series for $e^{1-\beta I}$ about an initial value β_0 , the model can be written

$$q = \alpha I e^{1-\beta_0 I} + \delta I^2 e^{1-\beta_0 I} + k \Delta y - r + e \quad (5)$$

which is linear in the unknown parameters α , δ , k and r .

- (ii) Starting with β_0 , estimates of these parameters (i.e., $\hat{\alpha}_1$, $\hat{\delta}_1$, \hat{k}_1 and \hat{r}_1) are obtained using Least Squares.
- (iii) β_0 is then replaced by $\beta_1 = \beta_0 - \hat{\delta}_1 / \hat{\alpha}_1$.
- (iv) The iteration (i.e., (ii) and (iii)) continues until the difference between $\hat{\beta}_k$ and $\hat{\beta}_{k-1}$ is very small, i.e., $\hat{\delta}_k$ is less than a prespecified small value. At this stage the values of $\hat{\alpha}$, $\hat{\beta}$, \hat{k} and \hat{r} are taken as $\hat{\alpha}_k$, $\hat{\beta}_k$, \hat{k}_k and \hat{r}_k .

• Model 3

Another model considered in the present work is obtained by replacing $f(I)$ in equation (2) by a saturation model (i.e., it does not take photoinhibition into account), which has been used by Smith (1936).

This leads to

$$q = \alpha \frac{I}{\sqrt{1 + \beta I^2}} + k \Delta y - r + e \quad (6)$$

Estimation of the parameters of the model

The parameters of the model, which are: α , β , k and r can be estimated by using the following algorithm:

- (i) Expansion of the first term in the right-hand side of equation (6) in a first-order Taylor series about an initial value, β_0 , of β and substitution of the resulting approximation into (6) gives:

$$q = \alpha \frac{I}{\sqrt{1 + \beta_0 I^2}} + \delta \frac{I^3}{2\sqrt{1 + \beta_0 I^2}^3} + k \Delta y - r + e \quad (7)$$

which is linear in the unknown parameters α , δ , k and r . Steps (ii), (iii) and (iv) are exactly the same as used for model 2.

• Model 4

Another photoinhibition model is obtained by replacing $f(I)$ in equation (2) by Vollenweider's formula (Vollenweider, 1965). This gives:

$$q = \alpha \frac{I}{\sqrt{1 + \beta I^2} \sqrt{1 + a^2 \beta I^2}} + k \Delta y - r + e \quad (80)$$

where α is a photoinhibition parameter which becomes 0 when photoinhibition does not occur.

Estimation of the parameters of the model

The procedure used for estimating the unknown parameters (i.e., α , β , a , k and r) is quite similar to those applied in the previous cases, though the calculations are more tedious. Thus,

- (i) The first term in the right-hand side of equation (8) is expanded in a first-order Taylor series about two initial estimates (i.e., α_0 and β_0) of α and β . Substituting the resulting approximation into (8) leads to:

$$q = \alpha \frac{I}{\sqrt{1 + \beta_0 I^2} \sqrt{1 + a^2 \beta_0 I^2}} + \delta \frac{I^3}{\sqrt{1 + \beta_0 I^2} \sqrt{(1 + a^2 \beta_0 I^2)^3}} + \gamma \frac{I^3}{\sqrt{(1 + \beta_0 I^2)^3} \sqrt{(1 + a^2 \beta_0 I^2)^3}} + k \Delta y - r + e \quad (9)$$

which is linear in the unknown parameters α , δ , γ , k and r .

- (ii) Starting with a_0 and β_0 , estimates of the parameters (i.e., $\hat{\alpha}_1$, $\hat{\delta}_1$, $\hat{\gamma}_1$, \hat{k}_1 and \hat{r}_1) are obtained using linear regression analysis.

(iii) a_0 and β_0 are then replaced by

$$\alpha_1 = \alpha_0 - \frac{\hat{\delta} - a^2 \hat{\gamma}}{\hat{\alpha} a_0 \beta_0} \text{ and } \beta_1 = \beta_0 - \frac{2\hat{\gamma}}{\hat{\alpha}}, \text{ respectively.}$$

and step (ii) is repeated on the basis of the new values a_1 and β_1 .

(iv) The iteration stops as soon as both the differences

$\hat{a}_k - \hat{a}_{k-1}$ and $\hat{\beta}_k - \hat{\beta}_{k-1}$ are very small, that is when

$\hat{\delta}^2_k + \hat{\gamma}^2_k$ is less than a prespecified small value. The

values of $\hat{\alpha}$, $\hat{\beta}$, \hat{a} , \hat{k} and \hat{r} are then taken as $\hat{\alpha}_k$, $\hat{\beta}_k$, \hat{a}_k ,

\hat{k}_k , and \hat{r}_k , respectively.

• Model 5

The dissolved oxygen concentration observed at a given time may be considered as an outcome of the previous recorded values for the light intensity (at least over a certain period of time). An appropriate model for describing this situation has been developed by Dhrymes (1971) and it is known as a model with geometrically distributed lags. Thus, in equation (2) $f(I_k)$ is replaced by

$$p_t = \alpha \sum_{i=0}^{+\infty} \rho^i I_{t-i},$$

where I_{t-i} is the light intensity at time $t-i$ and ρ is the unknown lag parameter of the model. When the values I_{-i} ($i=0,1,\dots$) are unknown, one can eliminate them from the model by introducing the additional parameter w , which is given by $w = \alpha \sum_{i=0}^{+\infty} \rho^i I_{-i}$.

Hence, model (2) can be rewritten as

$$q_t = w\rho^t + \alpha \sum_{i=0}^{t-1} \rho^i I_{t-i} + k \Delta y_t - r + e \quad t=1,2,\dots,n \quad (10)$$

Note that when ρ is known, this is a linear regression model, but since the lag parameter ρ is unknown in the present case, the model is only partially linear. The procedures developed by El-Shaarawi (1977) and Shah and El-Shaarawi (1980) can be used for estimating the parameters w , α and ρ and calculating their exact confidence intervals at a given probability level.

Estimation of the parameters of the model

To find \hat{w} , $\hat{\alpha}$ and $\hat{\rho}$,

- (i) we linearize the expression of q_t by expanding ρ^t in a first-order Taylor series about an initial estimate ρ_0 ; this leads to

$$q_t = w\rho_0^t + \alpha \sum_{i=0}^{t-1} \rho_0^i I_{t-i} + \delta [w t \rho_0^{t-1} + \alpha \sum_{i=0}^{t-1} i \rho_0^{i-1} I_{t-i}] + k \Delta y_t - r + e$$

where $\delta = \rho - \rho_0$ and $t=1,2,\dots,n$ (11)

(ii) For a given value of ρ (e.g., $\rho=0.5$), estimates \hat{w}_0 and $\hat{\alpha}_0$ for w and α are obtained from (10) using linear regression analysis.

(iii) We next consider model

$$q_t = w \rho_0^t + \alpha \sum_{i=0}^{t-1} \rho_0^i I_{t-i} + \delta \left[\hat{w} \rho_0^{t-1} + \hat{\alpha}_0 \sum_{i=0}^{t-1} i \rho_0^{i-1} I_{t-i} \right] + k \Delta y_t - r + e$$

which is linear in w , α , δ , k and r (12)

- (iv) This gives new estimates \hat{w}_1 , $\hat{\alpha}_1$, and $\hat{\delta}_1$ for w , α and δ , respectively.
- (v) In model (12) $\hat{\rho}_0$, \hat{w}_0 and $\hat{\alpha}_0$ are then replaced by $\hat{\rho}_1 = \hat{\delta}_1 + \hat{\rho}_0$, \hat{w}_1 and $\hat{\alpha}_1$, respectively, and regression analysis is repeated.
- (vi) The procedure stops as soon as $\delta_k = \rho_k - \rho_{k-1}$ is smaller than a prespecified value and the estimates of w , α , ρ , k and r are then taken as \hat{w}_k , $\hat{\alpha}_k$, $\hat{\rho}_k$, \hat{k}_k and \hat{r}_k , respectively.

It must be emphasized that all the models are interrelated: for example, if $a = 0$ in model 4, we obtain model 3 and if $\beta = 0$ in model 2 or model 3, then we reach the linear model (i.e., model 1). Moreover, model 1 is also a special case of model 5 since equation (10) simplifies to equation (3) when ρ is set equal to zero. Further, note that when $I = 0$ there is no production and models 1, 2, 3 and 4 reduce to

$$q = k \Delta y - r + e \quad (13)$$

This offers a very simple way for assessing the parameters k and r . Hence, from equation (2) it can be stated that the production at stage t is then given as $p_t = q_t - \hat{k} \Delta y_t + \hat{r}$. Thus, the type of the relationship between the production and the light intensity ($P - I$ curve) can be evaluated graphically from the plot of p_t versus I_t .

RESULTS AND DISCUSSION

The raw data from Canagagigue Creek for the study period are presented in Figure 1, which shows the temporal variation of the oxygen concentration observed and the oxygen concentration at saturation, the light intensity and the temperature in parts a), b) and c), respectively. The saturation value of the oxygen concentration was calculated from the measured temperature and was corrected for 200 m elevation above sea level.

The component processes in the oxygen metabolism of a stream, i.e., the primary production, the oxygen exchange constant and the rate of respiration were determined by means of nonlinear regression analysis applied to a simple oxygen mass balance equation (see equation (1)). This approach is quite different from the cross-correlation computational technique developed by Schurr and Ruchti (1975) or the extended Kalman filter used by Cosby et al. (1984) to provide estimates of the model parameters. Thus, the algorithms presented in the previous section for modelling the rate of change of dissolved oxygen led to the following regression equations, which were obtained by specially written programs using APL computer system:

$$q = 0.215 \Delta y - 0.578 \quad (\text{equation 13})$$

$$q = 0.265 I + 0.250 \Delta y - 0.611 \quad (\text{model 1})$$

$$q = 0.246 I e^{1-0.149I} + 0.329 \Delta y - 0.870 \quad (\text{model 2})$$

$$q = 0.602 I/\sqrt{1 + 0.108I^2} + 0.328 \Delta y - 0.866 \quad (\text{model 3})$$

$$q = 0.651 I/\sqrt{1+0.180I^2}/\sqrt{1+0.004I^2} + 0.331\Delta y-0.879 \quad (\text{model 4})$$

$$q_t = 111.253 \times 0.001^t + 0.264 \sum_{i=0}^{t-1} 0.001^i I_{t-i} + 0.251 \Delta y - 0.611$$

$t = 1, \dots, n$ (model 5)

Figure 2 is a plot of the realized photosynthesis-light relationship for the first four models considered. The figure indicates that no distinct photoinhibition was observed within the range of light intensity that occurred during the data period. Models 2, 3 and 4 were generally representative of the photosynthesis-light behaviour, moreover the similarity of the photosynthesis-light responses for those models is apparent.

The estimates of the component parameters, the values of P_{max} , I_s and the slope (E_0) of the P-I curve as light intensity approaches zero are summarized in Table 1. The residuals, which are given in the last column of Table 1, permit a rough comparison of the relative goodness-of-fit for each model.

Table 1: Results of productivity analysis: parameter values and curve characteristics.

Models	E_0	p_{max} $gm^{-3}h^{-4}$	I_s $Em^{-2}h^{-1}$	k h^{-1}	r $gm^{-3}h^{-1}$	residuals
1	0.265	undefined	undefined	0.250	0.611	13.115
2	0.669	1.654	6.717	0.329	0.870	9.560
3	0.602	1.831	undefined	0.328	0.866	9.557
4	0.651	1.327	5.955	0.331	0.879	9.514
5 *		$\rho=0.001$		0.251	0.611	13.111

* Since model 5 did not show any improvement when compared to model 1 (which is a special case of model 5 when $\rho=0$), it was not considered any further.

A more convenient way for evaluating the relative goodness-of-fit is given in Figure 3, where both the observed and the predicted rates of changes of dissolved oxygen are plotted against time. This has been done for each model in Figure 3 a), b), c) and d), respectively. Any systematic difference between the two curves is due to the lack of fit of the model.

As can be seen in Figure 3 and from the residuals recorded in Table 1, model 1 (the linear model) does not fit the data very well. The proportion of the variance explained by this model is

approximately 45% ($R^2=0.45$). Further, the turning-points test (Kendall and Stuart, 1968) was used to test for the randomness in the series of residuals, in other words, the problem was to know if the series of residuals differs significantly from a random white noise sequence. The null hypothesis (i.e., randomness of the residuals) has been rejected at the 1% level for model 1, whereas the test was less significant for both models 2 and 3 ($P=0.0475$) and also model 4 ($P=0.0314$). Although none of the models can be accepted as strictly adequate, a substantial improvement is however obtained with models 2, 3 and 4 ($R^2=0.60$ for all three of them) when compared to model 1. Thus, the goodness-of-fit is quite parallel for those three models, which subsequently yielded very similar parameter values and curve characteristics especially for models 2 and 3 (see Figure 2 and Table 1). The close agreement between reaeration and respiration rates, which has been observed more particularly for models 2, 3 and 4, was expected since the processes of reaeration and respiration are explicitly independent of light or photosynthesis in the mass balance equation. Hence, any of the equations (4), (6) or (8) can be used for assessing the component rates of dissolved oxygen.

If the estimates of k and r calculated from equation (13) (i.e., when $I=0$) are taken into account, the reaeration and respiration rates calculated from all the regression equations considered fell in the range $0.22-0.33 \text{ h}^{-1}$ and $0.58-0.88 \text{ g m}^{-3}\text{h}^{-1}$, respectively. This is in agreement with the values observed by Cosby *et al.* (1984) for a small second-order stream in Denmark and also the values reported by Schurr and Ruchti (1975) for several Swiss rivers.

Further, with model parameters in hand, it becomes possible to distinguish and to assess separately the different components which interact to produce the daily curve of oxygen change. These components (i.e., production, diffusion and respiration) are embodied in the regression equation that describes the oxygen balance. Thus, the component processes in the oxygen metabolism for the study period were calculated from the fitted regression equations and the curves obtained for each model are given in Figure 4 a), b), c) and d), respectively. The combined effect of production (p), diffusion (d) and respiration (r) is given in the rate of change curve (q). These curves, which can be considered as characteristic of a given segment of flowing water at least over a specific period of time, can undoubtedly help to understand the mechanisms and the relative importance of the component processes in the oxygen metabolism. For example, it is of interest to note, as it clearly appears in the diffusion curve, that the exchange of oxygen with the air was not well balanced for the section of the stream studied since invasion was more important than outgassing. The work reported here showed, by means of an example, that regression analysis applied to nonlinear models provides an appropriate tool for carrying out the assessment of the component processes in the daily dissolved oxygen metabolism of a stream.

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FIGURES

Figure 1: Raw data from the Canagagigue Creek for the study period.

Figure 2: Photosynthesis-light responses using values of the parameters from models 1, 2, 3 and 4.

Figure 3: Plots of observed and fitted concentrations of dissolved oxygen against sequential order of the observations for the study period.

Figure 4: Component processes in the oxygen metabolism for the study period, calculated from the different models' regression equations.

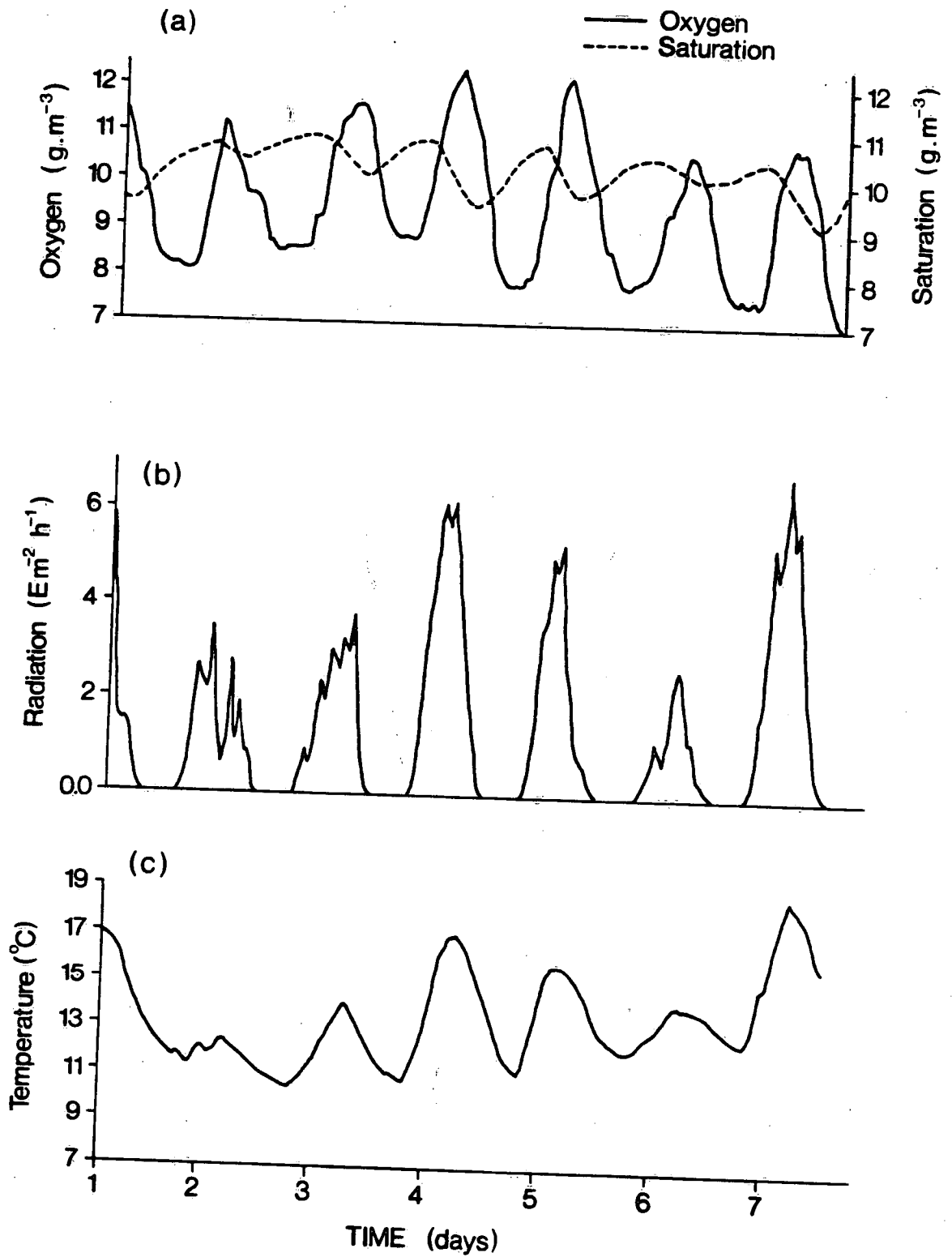


Figure 1. Raw data from the Canagagigue Creek for the study period.

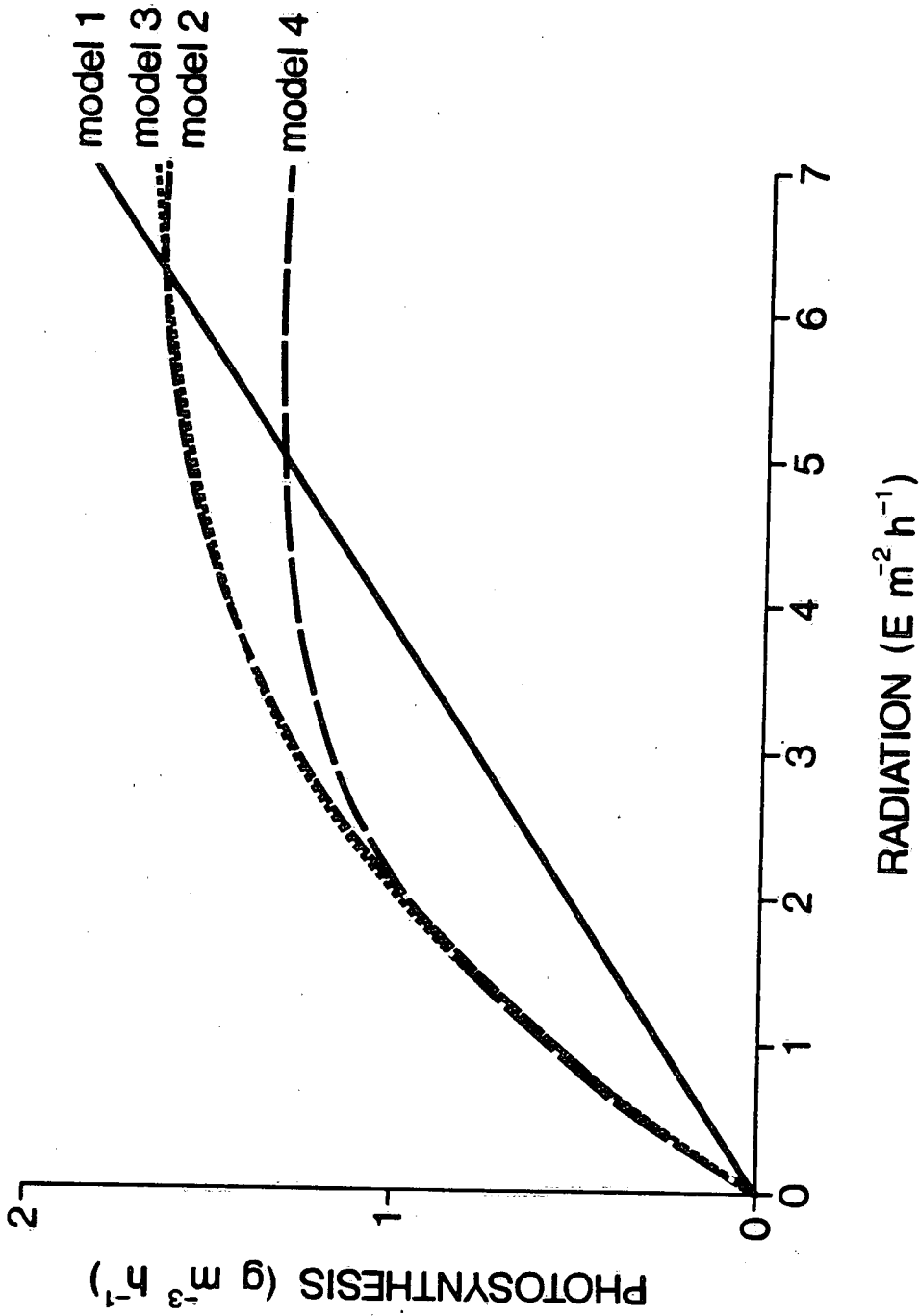


Fig 2: Photosynthesis - light responses of the first four models.

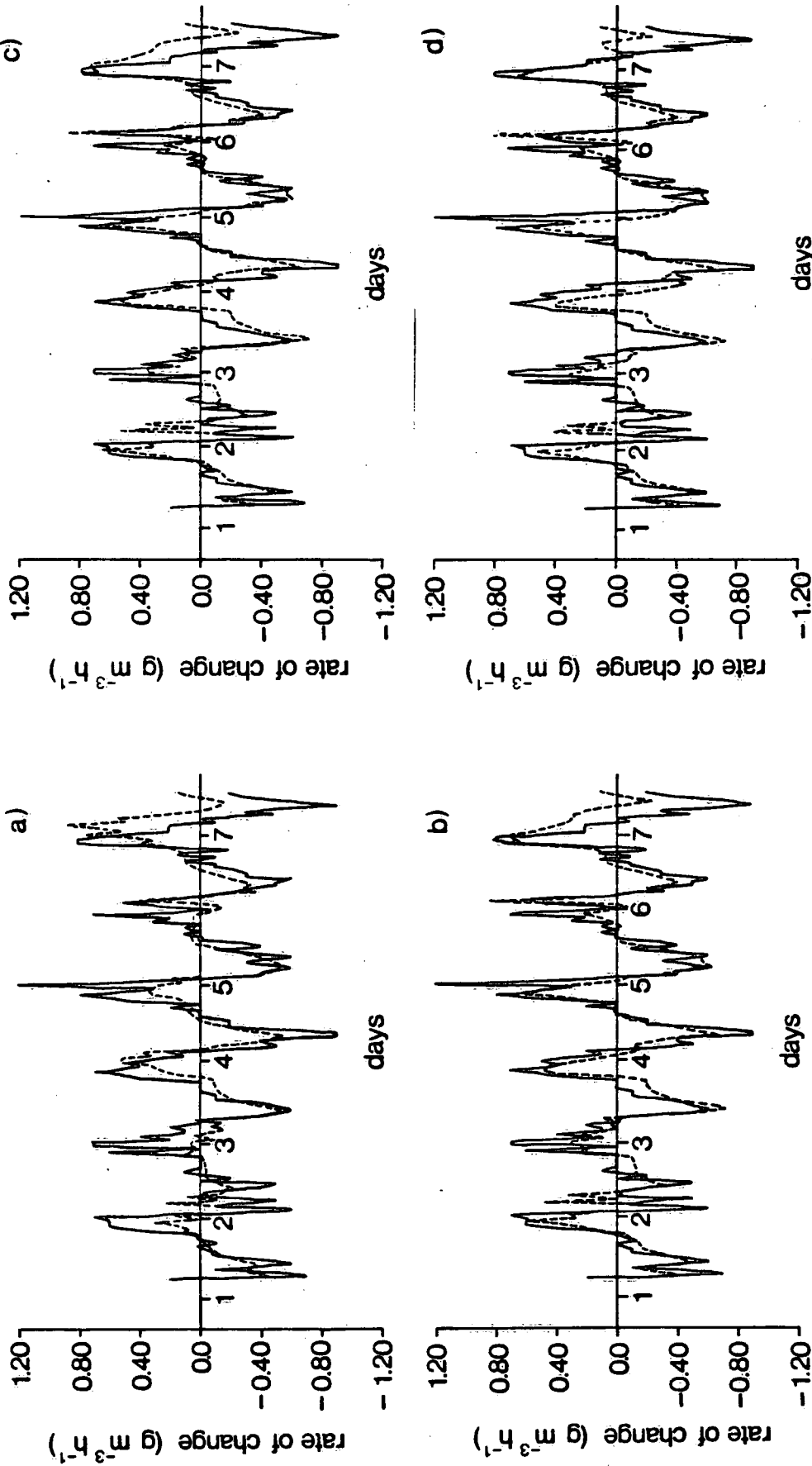


Figure 3: Plots of observed and fitted concentrations of dissolved oxygen against sequential order of the observations for the study period.

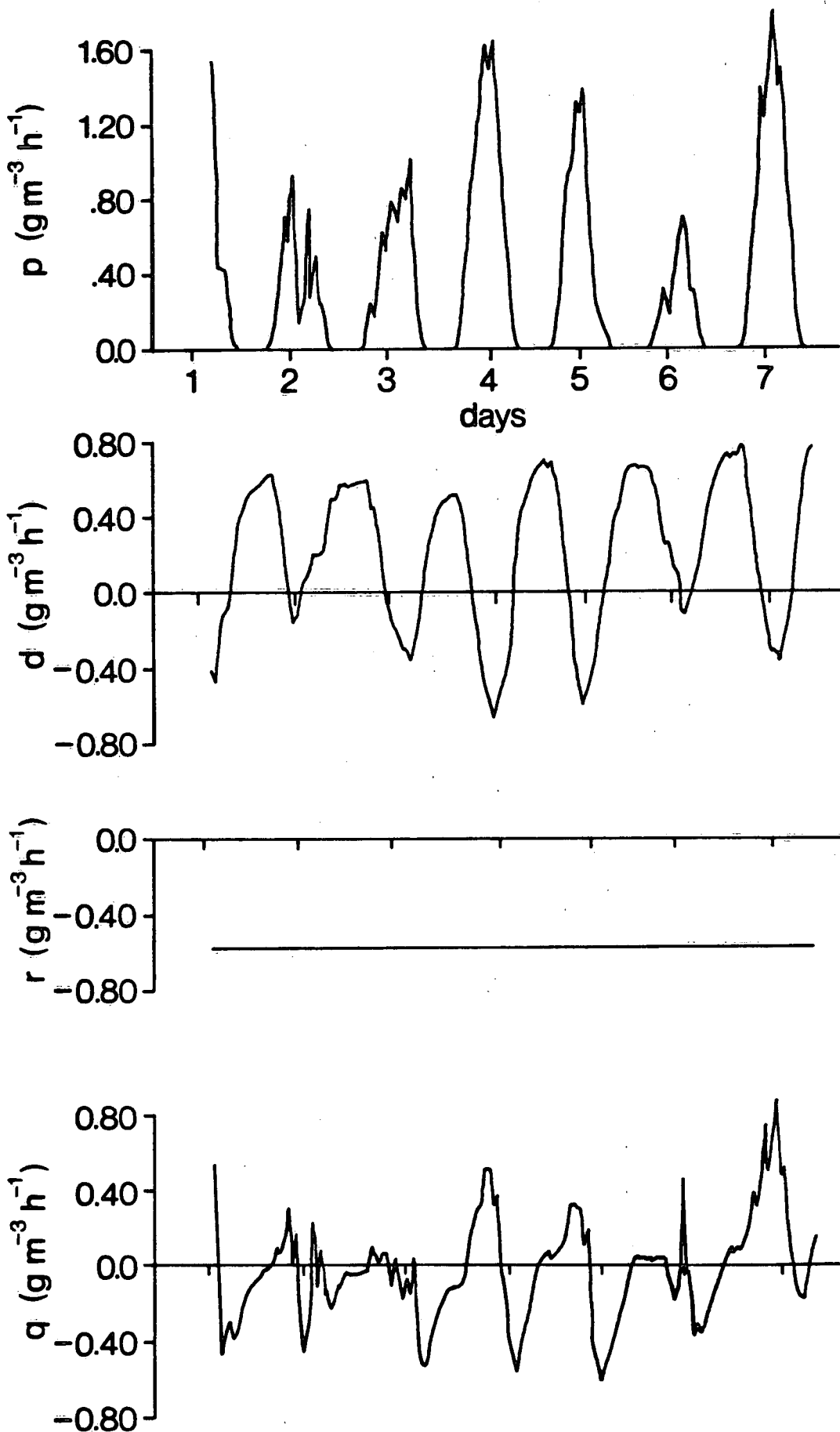


Fig. 4a : Component processes in the oxygen metabolism calculated from model 1.

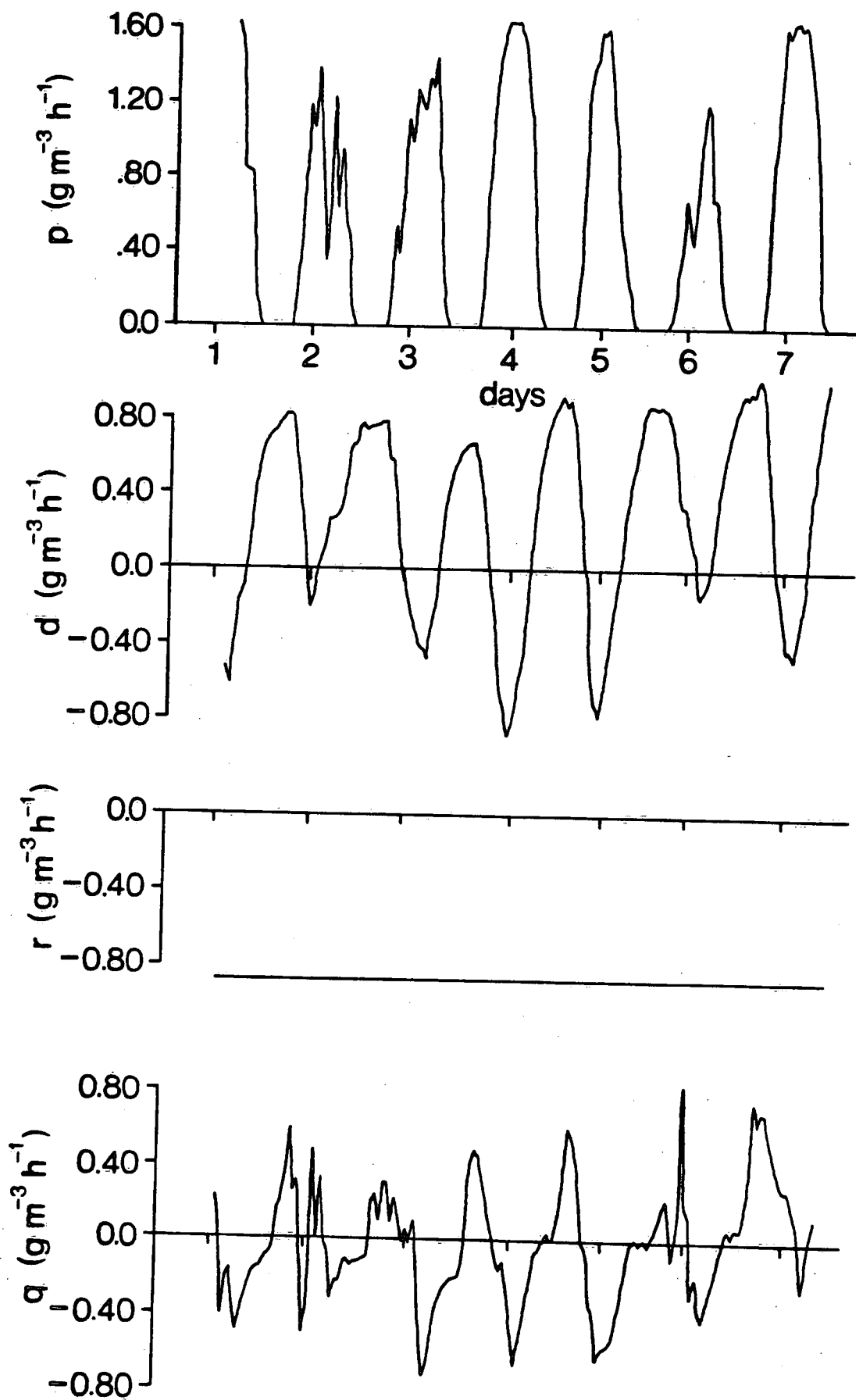


Fig. 4b: Component processes in the oxygen metabolism calculated from model 2.

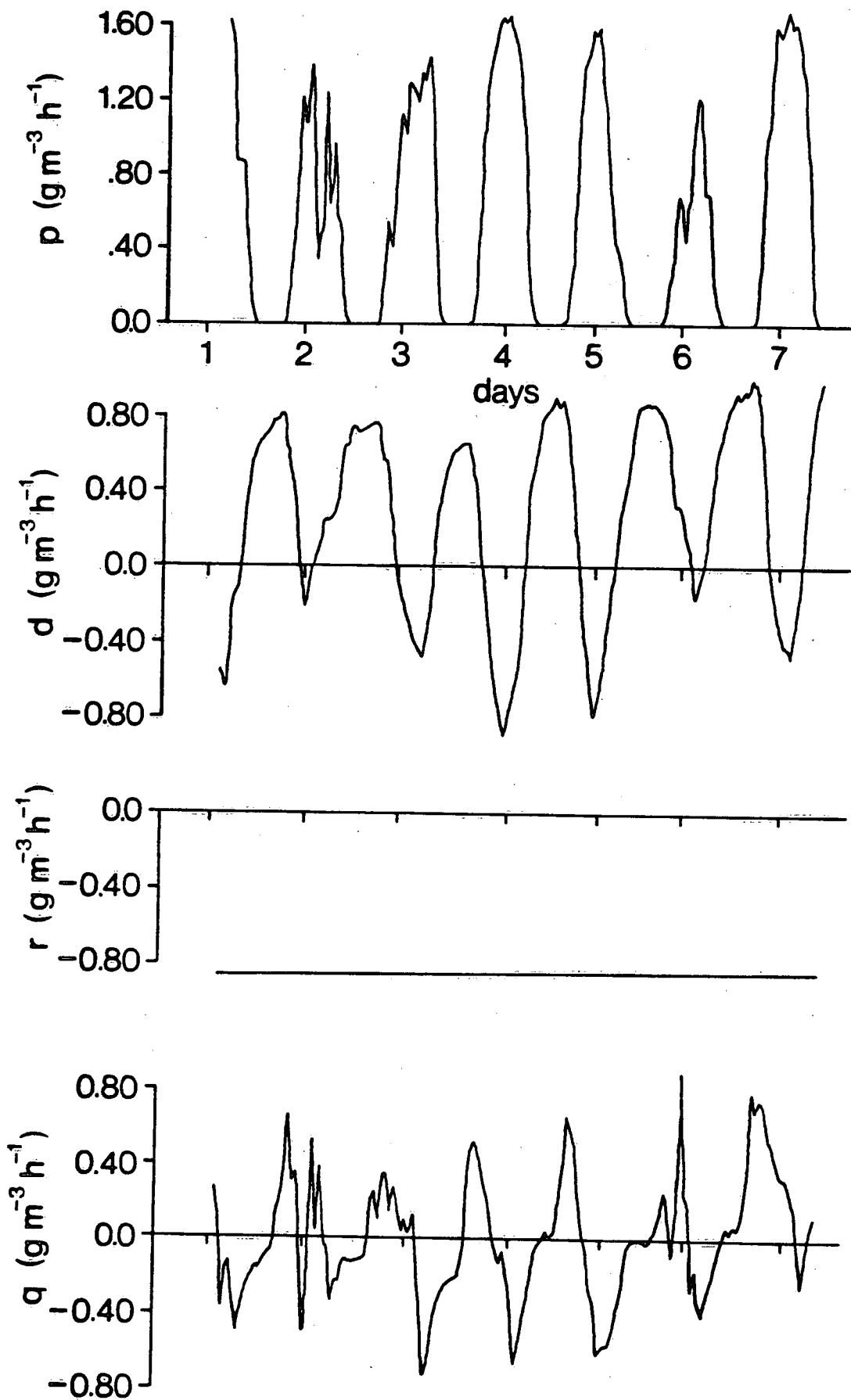


Fig. 4c: Component processes in the oxygen metabolism calculated from model 3.

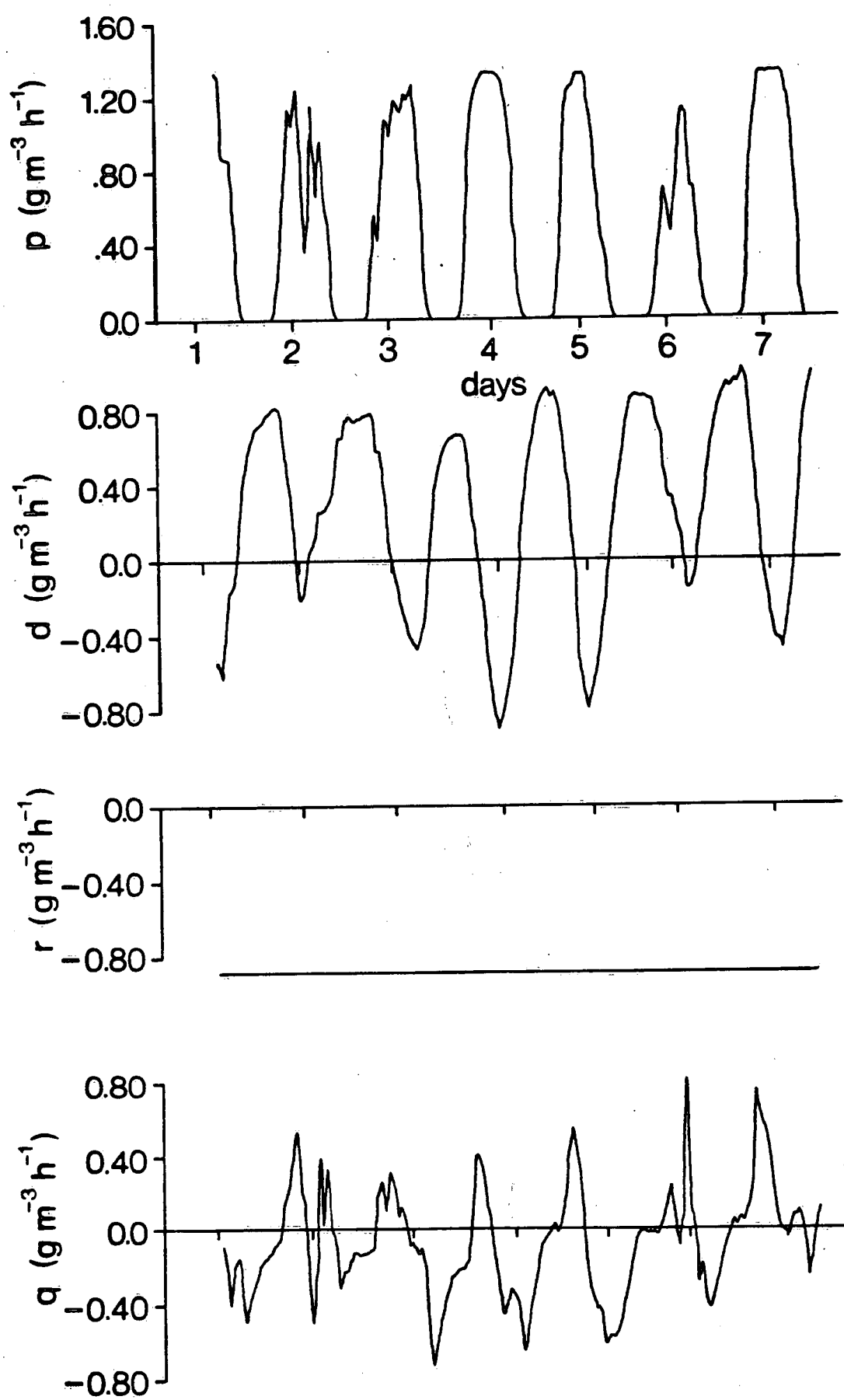


Fig. 4d: Component processes in the oxygen metabolism calculated from model 4.