

MODELLING THE DYNAMICAL EFFECT OF SOLAR RADIATION ON THE OXYGEN CONTENT OF A SMALL CREEK

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SUMMARY

Data from a small stream are used to explore various dynamical models of the oxygen level. Special attention is given to an analysis and a description of how the solar radiation affects the oxygen level. The models are formulated in continuous time using stochastic differential equations. The parameters of the models are estimated using discrete time data and a maximum likelihood method. The continuous time formulation makes it possible to directly interpret the parameters of the model, as the estimated parameters have specific physical, biological or chemical meaning. The advantages of using a low pass filter on the point measured solar radiation, as an input variable, are demonstrated. This investigation will eventually contribute to a comprehensive study of the dynamics that governs the oxygen content in a recipient. © 1998 John Wiley & Sons, Ltd.

KEY WORDS solar radiation; oxygen dynamics; time series analysis; dynamical modelling; low pass filter

1. INTRODUCTION

The variation of the oxygen content in aquatic systems like rivers is highly dependent on the variation of short wave radiation. About 44 per cent of the total radiation lies in the photosynthetic interval. Photosynthesis is a chemical reaction, by which plants in a river convert light energy into chemical energy. Production by photosynthesis and consumption from respiration take place in the water phase by phytoplankton, and by the macrophytes growing from the river bed.

The Gryde river is a small creek, located on the Danish Jutland peninsula. There is no biological oxygen demand exerted from organic matter in excess of natural levels and the agriculture surrounding the river is not expected to supply large amounts of oxygen consuming matter. Measuring stations were installed in the late 1970s and other data sets from this river have since been the subject of many studies (Thyssen *et al.* 1983; Erlandsen and Thyssen 1983; Jeppesen and Thyssen 1984; Cosby 1984; Cosby *et al.* 1984; Cosby and Hornberger 1984; Erlandsen and Sørensen 1984).

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The purpose of the present work is to investigate the photosynthesis as a function of solar radiation, as observed indirectly by the oxygen concentration. Eight different mathematical models for the photosynthesis–light relationship will be investigated.

The models have all been previously suggested (Thyssen 1980; Cosby 1984; Cosby *et al.* 1984). Seven of the models have been analysed in Cosby *et al.* (1984); however, the methods used in this paper are different. In their approach, a recursive estimation technique using an extended Kalman filter (EKF) (see Cosby and Hornberger 1984) was used to estimate the parameters. As pointed out by the authors, and demonstrated clearly in Ljung (1979), this technique is critically dependent on a correct specification of some variance parameters used in the EKF. The recursive estimates are used to construct average values/estimates of the parameters. Yet another method was presented by El-Shaarawi *et al.* (1988), who used a non-linear regression analysis approach via a Taylor series expansion. Five models were investigated in this work. The disadvantage of this method lies in the approximation that the Taylor series expansion represents.

In the present paper, a maximum likelihood method, described in Melgaard and Madsen (1993), is used to estimate the parameters of a continuous time, non-linear model. Compared to the methods used by Cosby *et al.* (1984) our method directly provides estimates of the parameters. Furthermore, a method is suggested for low pass filtering the solar radiation data. This filtering is suggested to compensate for the fact that the solar radiation is a very high frequency signal, which is probably measured some distance from the main body of the water. Therefore, only the low frequency part of the variation is expected to be representative. This is confirmed by the fact that the use of the filtered solar radiation as input leads to more precise parameter estimates and a considerably improved description of the variation of the oxygen content.

2. DESCRIPTION OF DATA

The data in this study were obtained several years after the previously mentioned studies were conducted. The aim is more concerned with the estimation of the physical parameters than with the performance of our estimation routine, as this has been tested on different kinds of physical models (see e.g. Madsen *et al.* 1990; Melgaard 1994; Melgaard *et al.* 1994; Jacobsen and Voss 1994; Jacobsen and Madsen 1996; Madsen and Holst 1995).

The data consist of measurements of oxygen, saturated oxygen, temperature and solar radiation, measured every 5 minutes during one week in June 1985 (see Figure 1). Here solar radiation is measured in langleys, symbol Ly, which is a non-standard unit used in many earlier studies. Today solar radiation is most frequently measured in W/m² per hour: Ly = cal/cm² = 41.868 kJ/m². Water depth is also measured, but is not explicitly involved in this model, as the depth is almost constant (about 73 cm) over the period. Also the cross-section of the river is fairly uniform. See Thomsen and Thyssen (1979), Thyssen *et al.* (1983) and Erlandsen and Thyssen (1983) for a description of the instrumentation and the experimental set-up.

3. FILTERING OF DATA

The solar radiation is measured as a point measurement, since it is obtained using one single solarimeter. This means that the variation of the solar radiation is dominated by high frequency variation, due to movements of clouds (Madsen *et al.* 1985).

In this paper it will be demonstrated that an improved description of the variation of the oxygen content in the river is obtained using low pass filtering of the solar radiation data instead

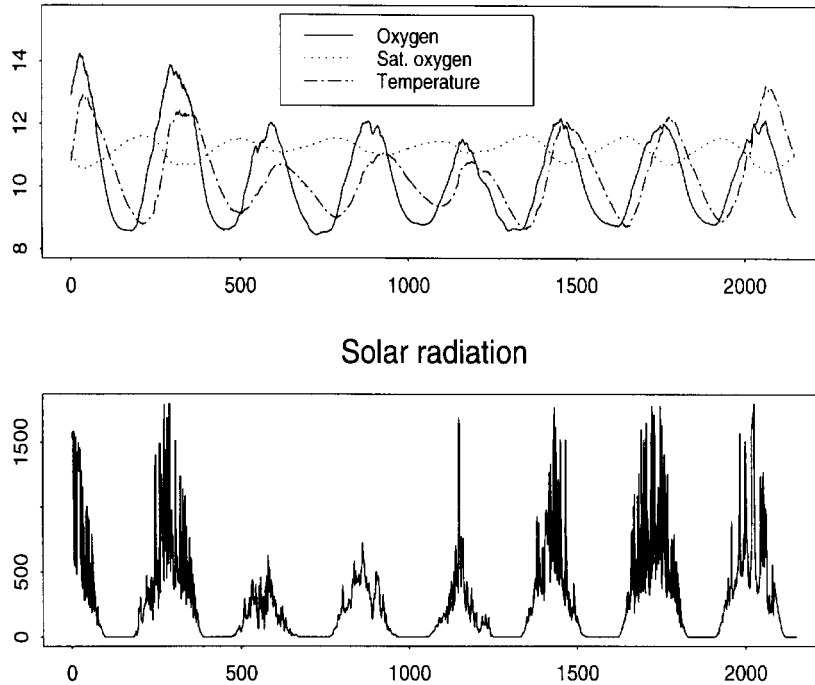


Figure 1. Measurements from Gryde river of the oxygen concentration and the saturated oxygen concentration (mg/l), the water temperature ($^{\circ}\text{C}$) and the solar radiation (Ly/min). The x -axis shows the time in 5 minute intervals

of the raw data themselves. There are several possible explanations for this. First of all, the photosynthesis may show some persistence, such that the irradiance to photosynthesis relationship must be a dynamic one. Secondly, the measurement of solar radiation does not take place along the element of water of interest: it is most likely to be measured some distance away from the position of the main body of the river. Therefore, the high frequency part of the variation is of no – or minor – relevance to the actual variation of the oxygen.

Depending on water quality, and how the solar radiation penetrates the water surface, the river may act as a low pass filter in itself. If this is the case it may not be correct to use the raw and unfiltered solar radiation data in the estimation procedure. The signal to noise ratio could obscure important dynamical information, thus making it more difficult to correctly estimate the parameters of the model. Hence, a low pass filtration of the solar radiation data should be performed.

The effects of considering a low pass filtered series of solar radiation as input is investigated by choosing a simple low pass filter. In further studies of models for the oxygen content in aquatic systems, we will consider the possibility of estimating an optimal low pass filter for the solar radiation.

3.1. A Low Pass Filter

An ideal low pass filter is a filter which only allows frequencies smaller than a given frequency to pass undisturbed, while holding back the higher frequencies. In practice, however, it is impossible to obtain the ideal low pass filter (Bloomfield 1976).

Kaiser and Reed (1977) suggest four different filter types that are all fairly simple and efficient. Of these, the so-called nearly equal ripple (NER) approximation, which is an approximation to the ideal low pass filter, is close to being the most efficient. It is characterized by nearly equal pass band and stop band magnitude errors.

For a discrete time series the filtered output data y_t are calculated by folding the original input data x_t with the impulse response function h for the filter, i.e.

$$y_t = \sum_{k=-\infty}^{\infty} h_k x_{t-k}. \quad (1)$$

This filter, however, requires an infinite input signal, which is not available in practice. Therefore only a span N_p of the filter weights is used at the expense of a less ideal filter. The folding equation thus reduces to:

$$y_t = \sum_{k=-N_p}^{N_p} h_k x_{t-k}, \quad (2)$$

where N_p is the number of terms after which the series is truncated. Kaiser and Reed (1977) suggest an odd number of terms to be used in the filter, chosen by $N = 2N_p + 1$, to avoid a half-interval time delay.

In Figure 2 different types of filters are shown. By increasing the number of terms N_p in the filter a steeper slope is obtained, and thereby a more ideal low pass filter. Simple averaging is frequently considered as a low pass filter. As indicated in Figure 2, averaging is far from the ideal low pass filter.

The NER filter uses the adjustable weighting function h_k , the effect of which is to reduce the error in size to $\pm \varepsilon$ at the expense of a slightly broadened transition band δ . This is accomplished by spreading the large approximation error at the band edge (resulting from series truncation) over the whole of the pass and stop bands. To design it, certain parameters have to be selected. In addition to the ones mentioned above (ε and δ) there is typically the band edge frequency β (see Figure 3).

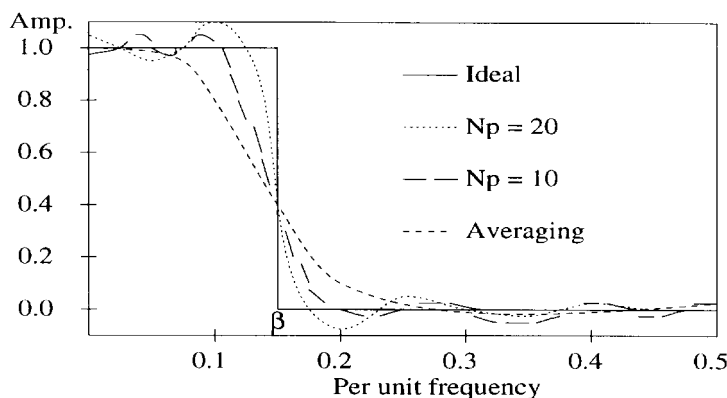


Figure 2. Characteristics for different type filters (Amp. is short for amplitude)

The approximation error ε , the transition band δ and the number of coefficients N_p are related by the design formula (Kaiser and Reed 1977):

$$N_p \approx (-20 \log_{10} \varepsilon - 7.95) / 28.72 \delta. \quad (3)$$

The filter is described in more detail in Kaiser and Reed (1977) and Jacobson and Voss (1992). In the present work the NER filter is used to filter the high frequency variations from the solar radiation data with the parameters: $N_p = 26$, $\varepsilon = 0.02$; $\delta = 0.035$ and $\beta = 1/12$ (according to the Shannon theorem). Figure 4 shows the time series of the solar radiation data after being filtered with the NER filter. A common use of the NER filter is to avoid aliasing when subsampling from a faster sampling interval. By using the filter one avoids folding the high frequencies into the sample Nyquist interval (Bloomfield 1976).

4. MODEL EQUATIONS

Most often the simple first order model, formulated by Odum (1956), is used for a description of the dynamics of the oxygen concentration in rivers:

$$\frac{dC}{dt} = K(C_m - C) + P(I) - R, \quad (4)$$

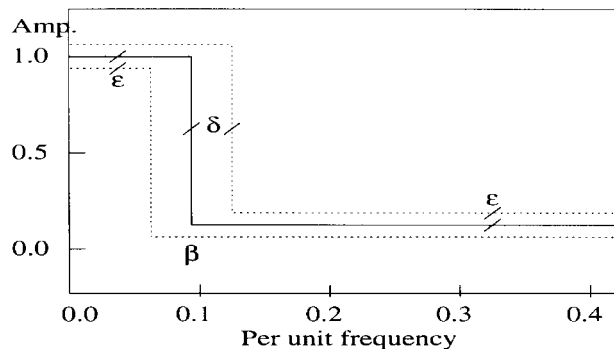


Figure 3. Design definitions for the parameters of the NER filter, where ε is the approximation error, δ is the width of the transition band and β is the band edge frequency

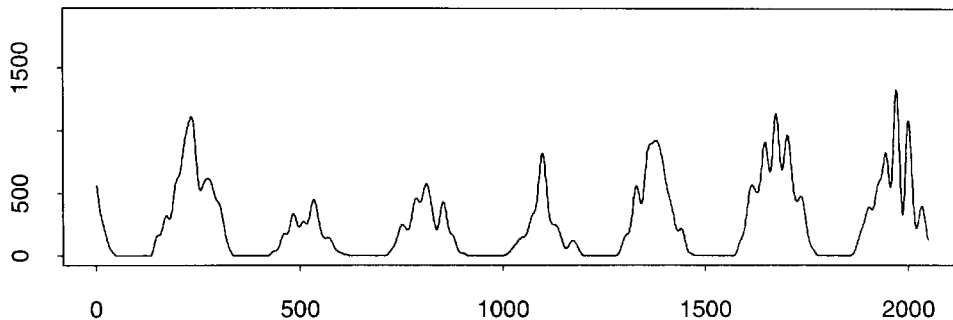


Figure 4. Solar radiation (Ly/min) data after using the NER filter with $\varepsilon = 0.02$, $\delta = 0.035$ and thus $N_p = 26$. The x -axis shows time in 5 minute intervals

where C is the oxygen concentration, C_m the saturated oxygen concentration (both in mg/l), K the reaeration constant (in h^{-1}), and R the respiration (in mg/l), while $P(I)$ (in mg/l) is the photosynthesis described as a function of solar radiation I (in Ly/min).

This model includes only the state of oxygen. The respiration was considered constant, while the photosynthesis was expected to vary in a diurnal sine-like fashion (solar radiation was not measured). Often solar radiation is not measured and therefore the photosynthesis is modelled by some empirical function, e.g. a sustained sunlight effect (see Young and Beck 1974; Beck and Young 1975; Whitehead and Young 1975; Whitehead 1980). Later studies (Thyssen *et al.* 1983; Erlandsen and Thyssen 1983; Jeppesen and Thyssen 1984; Cosby 1984; Cosby *et al.* 1984; Cosby and Hornberger 1984; Erlandsen and Sørensen 1984; El-Shaarawi *et al.* 1988) modelled the photosynthesis directly as a function of solar radiation.

In the models for photosynthesis, some physical parameters are introduced. Regardless of the exact function for the photosynthesis–light relationship, the following main parameters are introduced to characterize the relationship: the slope of the initial photosynthetic curve E_0 as the light intensity approaches zero, and the maximum photosynthetic rate P_m . The ratio E_0/P_m is the light intensity at which the line tangent to the initial slope intersects the line tangent to the maximum photosynthetic rate. The equations for eight different photosynthetic models (as a function of the measured solar radiation) are listed and depicted in Figure 5.

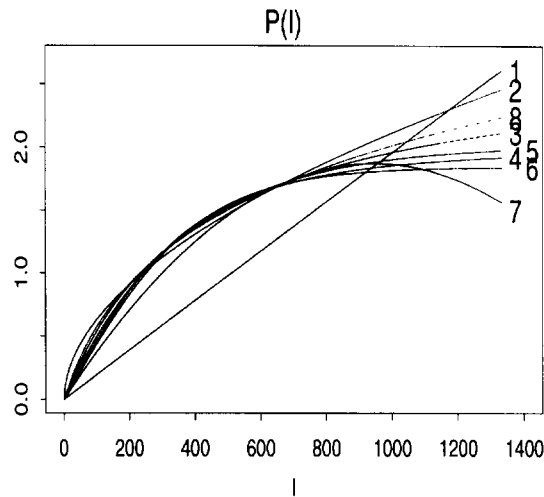


Figure 5. Equations for the eight photosynthetic models $P(I)$ as a function of the solar radiation. The unit for $P(I)$ is mg/l. The functions in the figure are shown with the parameter values estimated from the filtered solar radiation data

1. $P(I) = E_0 I$
2. $P(I) = E_0 I^2$
3. $P(I) = P_m \frac{1}{P_m/E_0 I + 1}$
4. $P(I) = P_m \frac{1}{\sqrt{(P_m/E_0 I)^2 + 1}}$
5. $P(I) = P_m (1 - \exp(-E_0 I/P_m))$
6. $P(I) = P_m \tanh(E_0 I/P_m)$
7. $P(I) = E_0 I (1 - E_0 I/P_m)$
8. $P(I) = P_m \ln(1 + E_0 I/P_m)$

4.1. Temperature Dependency

Some of the parameters in (4) are temperature dependent, namely the reaeration coefficient K , the respiration rate R and the photosynthesis light relationship $P(I)$. Typically they are modelled by exponential functions of the Arrhenius type:

$$K(T) = \kappa_{20} 1.0241^{T-20} \quad [\text{h}^{-1}] \quad (5)$$

$$R(T) = \rho_{20} 1.07^{T-20} \quad [\text{mg}/1] \quad (6)$$

$$P(T, I) = 1.035^{T-20} P(I) \quad [\text{mg}/1] \quad (7)$$

where the water temperature T is measured in degrees Celsius. The correction parameter 1.07 for respiration was suggested by Simonsen (1974) and Erlandsen and Thyssen (1983), whereas the correction parameter 1.0241 for reaeration is found in Pedersen (1994) and the temperature correction for photosynthesis is 1.035 according to Thyssen (1980). Respiration from plants is specific to the type of plant and its habitat.

The differential equation (4) may then be rewritten as

$$\frac{dC}{dt} = AC + a \quad [\text{mg}/1], \quad (8)$$

where the terms (5), (6) and (7) are included, i.e.

$$A = -\kappa_{20} 1.0241^{T-20} \quad (9)$$

$$a = \kappa_{20} 1.0241^{T-20} C_m + 1.035^{T-20} P(I) - \rho_{20} 1.07^{T-20}. \quad (10)$$

Now the model is easily formulated as a state space model. The state space model furthermore contains a description of how the measurements are related to the oxygen concentration: see Jacobson and Madsen (1996) for details.

The parameters of the model are estimated using a program called CTLISM (see Madsen *et al.* 1990; Melgaard and Madsen 1993; Madsen and Holst 1995). This program is able to estimate embedded parameters in stochastic linear and non-linear differential equations. The program uses a maximum likelihood method where an extended Kalman filter is used in evaluating the maximum likelihood function (see Melgaard and Madsen 1993; Jacobsen and Madsen 1996).

Our implementation of the extended Kalman filter is quite different from that of Cosby and Hornberger (1984). In their approach the extended Kalman filter is used to obtain recursive estimates of the parameters by including the parameters in a state vector. Final parameter estimates are obtained by averaging the recursive estimates. Their approach requires a reasonable prior specification of noise covariances for the state variables. This is a rather difficult task, and furthermore it is well known from Ljung (1979) that divergence of the parameter estimates can be traced to misspecification of the state noise covariance. Also, the method suggested by Cosby and Hornberger (1984) does not incorporate any temperature dependence of the parameters.

In our work we estimate the parameters directly and we avoid extending the state vector and the intermedium recursive estimates. Also the noise covariance are estimated along with the parameter estimates; hence the potential for misspecification of noise is avoided. The extended Kalman filter is solely used to obtain the one-step predictions which enter the likelihood function (Jacobsen and Madsen 1996). Finally, the method is quite simple to use.

5. RESULTS AND DISCUSSION

Tables I and II show the estimated parameters and their standard variations for all the models and for unfiltered and filtered solar radiation, respectively. The variance of the simulation error is denoted by σ_{sim}^2 .

Cosby *et al.* (1984) found reaeration coefficients in the range 0.25–0.45 h⁻¹. This was for data from 1978, from five measuring stations with 12 weekly data sets from February to October. El-Shaarawi *et al.* (1988) found reaeration coefficients in the range 0.25–0.33 for a Canadian river. This compares very well with our estimates.

In order to compare the models we introduce the R^2 value as the ratio of the difference between the variance and the simulation error to the variance:

$$R^2 = \frac{V[Y] - V[Y - Y_{sim}]}{V[Y]}, \quad (11)$$

where for the actual data, the variance $V[Y] = 1.8218$. It is seen in Tables I and II that the simulation performance for most of the models is nearly the same, with models 3, 4, 5 and 8 almost identical. Of these, model 8 is selected to show simulations and residuals (Figure 6).

Considering the individual parameters it must be recognized that E_0 and P_m have a different interpretation for the different models, but the values of ρ_{20} and κ_{20} can be compared for all models.

It is seen from Table I that, apart from the linear model 1 and to some extent model 7, the values of ρ_{20} and κ_{20} are the same if we take into account the uncertainty of the estimates. For the filtered case it is seen that the values of ρ_{20} and κ_{20} are slightly higher and the precision of the parameter estimate is much better. We attribute the difference in all the parameter estimates to the larger uncertainty associated with the unfiltered data.

Table I. Parameter estimates for unfiltered data: standard deviations are shown in parentheses

Model	E_0 ($\frac{\text{mgO}_2/\text{l h}}{\text{Ly/min}}$)	P_m ($\text{mgO}_2/\text{l h}$)	α	ρ_{20} ($\text{mgO}_2/\text{l h}$)	κ_{20} (h^{-1})	σ_{sim}^2	R^2
1	0.138×10^{-2} (0.403×10^{-4})	–	–	0.802 (0.026)	0.204 (0.758×10^{-2})	0.552	0.698
2	0.761×10^{-1} (0.688×10^{-2})	–	0.468 (0.013)	1.450 (0.035)	0.297 (0.785×10^{-2})	0.207	0.887
3	0.675×10^{-2} (0.329×10^{-3})	2.678 (0.076)	–	1.431 (0.030)	0.305 (0.695×10^{-2})	0.199	0.892
4	0.458×10^{-2} (0.173×10^{-3})	2.045 (0.049)	–	1.393 (0.031)	0.303 (0.744×10^{-2})	0.206	0.888
5	0.549×10^{-2} (0.209×10^{-3})	2.050 (0.051)	–	1.405 (0.030)	0.304 (0.726×10^{-2})	0.204	0.888
6	0.425×10^{-2} (0.155×10^{-3})	1.895 (0.046)	–	1.372 (0.031)	0.300 (0.783×10^{-2})	0.212	0.884
7	0.339×10^{-2} (0.918×10^{-4})	8.314 (0.183)	–	1.244 (0.030)	0.283 (0.770×10^{-2})	0.256	0.348
8	0.883×10^{-2} (0.580×10^{-3})	0.761 (0.033)	–	1.439 (0.031)	0.304 (0.736×10^{-2})	0.198	0.892

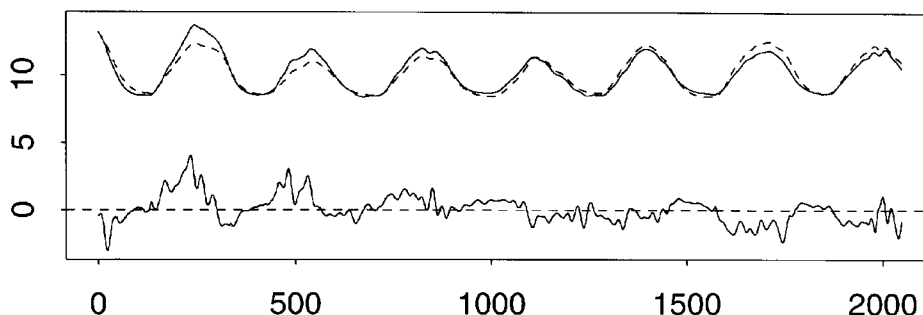


Figure 6. Time series of measured and simulated oxygen (in mg/l) plus prediction errors for model 8 (the logarithmic model)

In Figure 5 it is seen that several of the functions are almost indistinguishable. For both the filtered and unfiltered cases the best (simulation) fit was observed for models 3 and 8. Model 3 is a Michaelis–Menten type model advocated by for instance Erlandsen and Thyssen (1983) and Erlandsen and Sørensen (1984). The latter, however, then went on to simplify further to a linear model, which is seen here to give a significantly less adequate fit. Erlandsen and Thyssen (1983) find the logarithmic function (model 8) to give the best overall fit, although it is closely followed by model 3. A Michaelis–Menten reaction (model 3) is an enzymatically controlled function that assumes a constant enzymatic activity. As an approximation it captures the essence of a linear growth towards a saturation point.

A comparison of the filtered and unfiltered parameter estimates for model 3, along with the estimates from Pedersen (1994), is shown in Table III. Standard deviations for their estimates are not available. Erlandsen and Thyssen (1983) do not report their parameter estimates, as that paper concentrated more on estimating the temperature dependency parameter

Table II. Parameter estimates for filtered data: standard deviations are shown in parentheses

Model	E_0 ($\frac{\text{mgO}_2/\text{lh}}{\text{Ly}/\text{min}}$)	P_m ($\text{mgO}_2/\text{l h}$)	α	ρ_{20} ($\text{mgO}_2/\text{l h}$)	κ_{20} (h^{-1})	σ_{sim}^2	R^2
1	0.196×10^{-2} (0.310×10^{-4})	–	–	1.084 (0.018)	0.272 (0.526×10^{-2})	0.396	0.783
2	0.563×10^{-1} (0.319×10^{-2})	–	0.525 (0.083)	1.560 (0.019)	0.332 (0.415×10^{-2})	0.189	0.897
3	0.671×10^{-2} (0.181×10^{-3})	2.772 (0.049)	–	1.532 (0.014)	0.335 (0.526×10^{-2})	0.177	0.903
4	0.475×10^{-2} (0.100×10^{-3})	2.016 (0.027)	–	1.500 (0.017)	0.336 (0.403×10^{-2})	0.179	0.902
5	0.570×10^{-2} (0.130×10^{-3})	2.027 (0.029)	–	1.514 (0.018)	0.336 (0.404×10^{-2})	0.180	0.902
6	0.446×10^{-2} (0.951×10^{-4})	1.847 (0.024)	–	1.486 (0.018)	0.335 (0.426×10^{-2})	0.183	0.900
7	0.396×10^{-2} (0.622×10^{-4})	7.500 (0.089)	–	1.413 (0.017)	0.325 (0.424×10^{-2})	0.217	0.881
8	0.822×10^{-2} (0.301×10^{-3})	0.852 (0.024)	–	1.541 (0.018)	0.336 (0.408×10^{-2})	0.178	0.902

Table III. Comparisons of model 3. Standard deviations are shown in parentheses, but are not available for the prior estimated parameters in the photosynthetic function

Model 3 Variation	E_0 ($\frac{\text{mgO}_2/\text{1 h}}{\text{Ly/min}}$)	P_m ($\text{mgO}_2/\text{1 h}$)	ρ_{20} ($\text{mgO}_2/\text{1 h}$)	κ_{20} (h^{-1})
Unfiltered	0.675×10^{-2} (0.330×10^{-3})	2.676 (0.083)	1.428 (0.032)	0.300 (0.758×10^{-2})
Filtered	0.671×10^{-2} (0.181×10^{-3})	2.016 (0.052)	1.536 (0.018)	0.336 (0.526×10^{-2})
Pedersen (1994)	0.539×10^{-2} —	3.606 —	1.464 —	0.320 —

from the respiration. Therefore the comparison is done for model 3 only. No comparison is done with the results from El-Shaarawi *et al.* (1988), as their study did not include model 3.

Considering the estimated models in Figure 5 and the simulation performance for the various models, it is concluded that all the monotone and concave functions give a reasonable description of the photosynthesis–light relation.

5.1. Suggestions for Improvements

The models investigated here were very simple models that did not take phenomena into account other than reaeration, photosynthesis and respiration. There may be other physical processes related to rivers that influence the oxygen content.

Benthic organisms may have a significant influence, as shown by Thyssen (1982). Whitehead (1980) and Boyle and Scott (1984). The latter two papers reported an investigation from a small river in southern England, quite similar to Gryde river.

While light intensity may be the most important variable for the photosynthesis, there is also a dependency on carbon dioxide (CO_2), the water level and possibly the oxygen concentration. The CO_2 originates from the carbon system and is related to pH.

With respect to plants, there are two theories. Endogenous reactions in the plants involve consumption of CO_2 . When the pools are full, there is, loosely speaking, no need to keep up the same rate. This results in a lower rate of photosynthesis in the afternoon. The other theory encompasses the fact that pH is higher in the afternoon as the temperature rises. This would also cause changes in the CO_2 levels, thereby changing the rate of photosynthesis in the afternoon. Documentation for these theories is scarce outside the laboratory and the data available for the present study do not make it possible to identify these differences.

It is clear that, in order to obtain a series free of disturbing high frequency noise, without destroying important information in the data, a low pass filter should be applied. Here an available low pass filter was used. In further work the possibility of estimating an optimal low pass filter for the solar radiation will be considered.

Only a small set of new data was available for the present study. In order to obtain more prominent conclusions, more data sets from the same, and other, rivers should be investigated. For the present set of data, it is for instance not known what the reason for the large oscillations during the first two days might be. A respiration function solely dependent on temperature may ignore the effect from the oxygen concentration itself, inhibiting matter, plant types and light intensity (Simonsen 1974).

6. CONCLUSION

Several photosynthetic models as a function of solar radiation data were compared. The investigation was performed by estimating the parameters in stochastic differential equations. Both unfiltered and low pass filtered solar radiation data were used as input, and it is concluded that

1. The monotone and concave functions gave the best results and led to nearly the same estimates of the reaeration and respiration temperature coefficients.
2. A low pass filtering of the solar radiation data gave more precise parameter estimates.
3. Investigation of more data sets is necessary to obtain a better understanding of the photosynthetic relationship and whether other phenomena should be included in models for aquatic systems.

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