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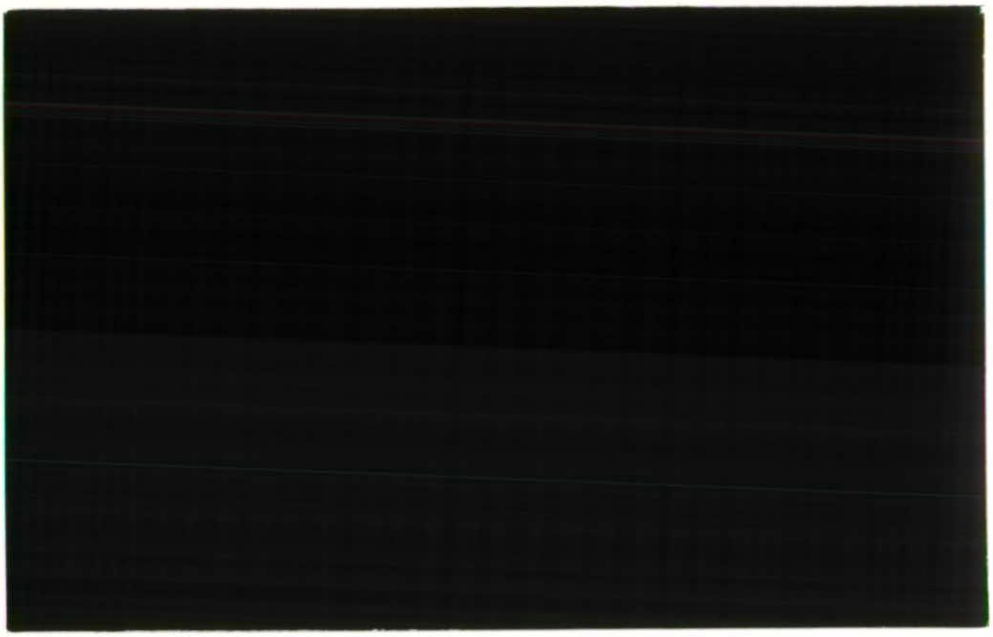

Natural Environment Research Council

A STUDY OF ALGAL MODELLING

The development and application
of a general algal model in Quasar

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Summary

This report describes the development of an algal model for inclusion in the water quality model Quasar. Modelling algae is an important tool in describing algal behaviour and predicting algal blooms. The term 'algae' describes small unicellar organisms capable of photosynthesis. Phytoplankton, or planktonic algae, are the suspended algae in the water column, and include cyanobacteria or blue-green algae.

The controlling factors for algal growth are light, nutrients and temperature. In most water systems in the U.K. nutrients are not limiting. Algal growth is then limited by light and temperature only. Algal loss factors are death, sedimentation and grazing.

In the model light limitation for algal growth is described with Steele's equation, integrated over depth with Lambert-Beer's extinction law. Self-shading of the algae is defined in the extinction factor. Temperature limitation is described with the Arrhenius expression. If nutrients are limiting, this limitation is described with Monod kinetics. Loss factors are described with a linear dependency on the chlorophyll-a concentration. The following parameters need to be calibrated in the model: growth rate, loss rate, optimum solar radiation and background extinction coefficient.

The algal model is tested with a data set of 3 years (1974-1976) weekly measurements of chlorophyll-a, flow, temperature and solar radiation at 6 sites along the Thames, forming 5 reaches. QSAR, a pre-version of Quasar, is used to test the model. The model parameters are calibrated for each reach separately with the 1974 data set. The fit of the model with the observed data is tested with R_t^2. Values for R_t^2 vary from 0.653 (reach 1) to 0.945 (reach 5). Reach 2 and 3 are calibrated with 2 parameter sets, to describe the spring bloom and summer bloom separately. Validation of the parameters with the 1975 and 1976 data sets is difficult. The model is found to be only slightly sensitive to the background extinction coefficient, whereas it is more sensitive to the growth and the loss rate parameters.

The algal model as described here can give an adequate representation of reality when incorporated in an integrated water quality model. It can give a good prediction of chlorophyll-a concentration in the River Thames, some peaks are under- or overestimated. Upstream conditions are mainly responsible for the timing of the peaks, the parameters have mainly an influence on the concentration of the peaks. It is a general algal model, it is not aimed to be the most detailed algal model possible. Phytoplankton is described as chlorophyll-a, the parameters describe average algal variation.

When the algal model is incorporated in Quasar, the following recommendations are made: The background extinction coefficient can be a fixed value, the model is not very sensitive to this parameter. Further research on the description of the solar radiation in Quasar is necessary. The development of a phosphate model in Quasar is necessary.

Preface

This report is the result of a 5 month research project in Water Quality Management undertaken at the Institute of Hydrology, as part of my course in Environmental Sciences at the Agricultural University, Wageningen (the Netherlands). The research contributed to the LOIS project, and was financed by it.

I wish to thank my supervisors at IH, Paul Whitehead and Doug Lewis, and my long-distance supervisor Hans Aalderink. E-mail proved to be a useful communication tool. I also wish to thank Richard Williams for further help with Quasar.

Not reflected in this report is the time I needed to learn how to program in Fortran; writing the Fortran code, and the compiling into executable files. The agony when again the screen filled itself with error messages. We got it working in the end, so I could run `my' model, which I did for about a thousand times!

I started with a healthy scepticism towards ecological modelling, and this attitude has been thoroughly reinforced by my experiences. This scepticism didn't prevent me from learning a great deal here, and not just about modelling. I have had a very good time at IH, I really felt part of the Water Quality Systems section, and of the social structure of IH. I want to thank everybody for the useful (?) discussions, good time, fun, pros and cons of running and cricket, running in lunchtime. I learned that not only algae flourish in the Thames, the Dutch rowing contingent did OK as well.

Marieke

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1 Introduction

In the last decade a number of models have been developed to model algal concentrations in water systems. This report describes the development of an algal model for inclusion in Quasar (QUAlity Simulation Along Rivers), a water quality model for rivers, developed at the Institute of Hydrology. Modelling algae is important in describing algal behaviour and predicting algal blooms.

The term `algae' generally describes `primitive' autotrophs, small unicellar organisms capable of photosynthesis. Common characteristics of algae are their possession of chlorophyll-a, their ability to use water as H-donor in photosynthesis, and their ability to use an aquatic habitat for growth. Phytoplankton, or planktonic algae, are the suspended algae in the water column, and include the cyanobacteria or blue-green algae. In this report phytoplankton are referred to as `algae'.

In rivers the same algal species are found as in stagnant waters. The algal community is very dynamic, the timescale on which changes take place is small. Major functional groups of algae are diatoms, green algae and blue-green algae. Diatoms usually have their peak concentration in spring, green algae in early summer and blue-green algae in summer (Moss, 1980; Reynolds, 1984; Reynolds, 1992).

The development of the algal model is performed within the framework of LOIS, Land-Ocean Interaction Study, a multidisciplinary study in which several institutes of the National Environmental Research Council collaborate. One of the research aims of the River Basins element is to determine land-to-sea fluxes of biological matter. Models like Quasar are important tools in the research (NERC, 1992).

In Quasar, algae are presently described using a constant concentration per month, involved in the dissolved oxygen equations. The aim of this study is to develop a general algal model, which is able to describe seasonal chlorophyll-a fluctuations.

The development of the algal model involves the following aspects. Firstly a literature review on algal behaviour and blooms, followed by a review of the mathematical descriptions of algal growth and loss processes, and interactions with dissolved oxygen concentration and biochemical oxygen demand. A study using available chlorophyll-a, flow and weather data is then made to test the developed model equations.

2 Theory

2.1 ALGAE IN RIVERS

2.1.1 Algal growth

Algae reproduce by cell division, with generation times of only hours or a few days (Moss, 1980). The controlling factors for algal growth are light, nutrients and temperature.

Light is an important factor, especially in waters with high nutrient loads where it is the limiting factor. When light intensities are insufficient to saturate instantaneous photosynthesis, it is unlikely that maximal growth rates will be reached (Reynolds, 1984).

The intensity, duration and underwater attenuation of solar radiation combine with temperature to control the photosynthetic production, increase in daylight is the most likely factor initiating the onset of spring diatom growth (Lack, 1971). The availability of nutrients determine the extent to which photosynthetic potential is translated into new cell material. These processes are also modified by the effects of water movement and stability (Reynolds, 1980 a).

Photosynthesis can proceed over a wide range of light intensities, but becomes inhibited at high light intensities. At lower temperatures, light saturation occurs at lower levels of irradiance (Reynolds and Walsby, 1975). Self shading of algae occurs when algal concentrations are high enough to cause significant diminution of solar radiation throughout the water column.

The most important nutrients for algal growth are phosphorus and nitrogen. Phosphorus is often the first limiting nutrient. This is shown in experimentally-enriched waters, and related studies (Reynolds, 1980 a; Codd and Bell, 1985). As a nitrogen source, ammonia (NH_3) is preferred over nitrate (NO_3) (Reynolds, 1982; van Benschoten and Walker, 1984; Bingham *et al.*, 1984). Silica is an important trace element for diatoms, as it is used for skeleton growth. In most water systems in the U.K. nutrients are not limiting for algal growth (NRA, 1990). Planktonic diatoms can utilize nitrate at concentrations below 0.1 ($mg.l^{-1}$) and phosphorus concentrations of 1 ($\mu g.l^{-1}$) can still produce large crops of *Asterionella* (diatom) (Lack, 1971).

The nutrient concentration in the water is not necessarily the concentration available for the alga, since it ignores fluxes and the content in the algal cells. Many algae absorb and store more than their immediate needs when nutrients are freely available. This so-called luxury consumption may be sufficient for an alga to continue to grow (two or three cell

divisions), despite nutrient exhaustion in the water. This is an explanation for the ability of blue-green algae to form a bloom when extreme nutrient deficiency has set in (Reynolds and Walsby, 1975).

Temperature is an important factor for the kinetics of biological processes. Maximum growth rates are dependent on temperature. Different species of algae have different optimum temperature ranges. Most algae have their optimum growth rate in the range 20-25 °C. *Anabaena flos-aqua* (filamentous blue-green) starts growing at temperatures above 5 °C and has its optimum at 10-15 °C. *Microcystis aeruginosa* (colonial blue-green) has its optimum at 17-18 °C. *Oscillatoria rubescens* (filamentous blue-green) has its optimum < 12 °C, and is considered to be a cold stenotherm species (Reynolds and Walsby, 1975).

2.1.2 Algal loss

Loss factors of phytoplankton in terms of population dynamics are any processes which actively remove biomass (chlorophyll-a) from the part of the water body under consideration. The main loss processes are death and decomposition, sedimentation, grazing and hydraulic wash-out. They are all to some extent dependent on the algal concentration.

Death and decomposition: algal cells may die from a variety of causes. Deprivation of adequate light to support photosynthesis, nutrient deficiency, exposure to toxic substances (including those produced by other algae), infection by fungi, bacteria and viruses. The eventual effects of these influences vary with species, with season and with the physiological condition of the algae concerned. The various influences almost certainly interact.

Sedimentation losses: algal particles will sink through a water column if they are heavier than water and unable to restore their position by swimming or regulating their buoyancy. Or when they are no longer kept in suspension by the water movement (wind-generated Eddy-currents) (Moss, 1980). It is difficult to obtain reliable data on the actual sinking rates, because of the variations in algal size and shape.

Grazing: phytoplankton is grazed by herbivores, zooplankton (such as the water flee *Daphnia*) and by larger invertebrates. Larger algae are relatively immune from grazing. This can explain why they are frequently dominating. Grazing has been the implicit subject of many studies in recent years, however the overall picture is still far from clear. Available data sometimes conflict with the widespread preconception that grazing necessarily `controls' the population stock.

Hydraulic washout: in a river system it is expressed as the balance between upstream concentration, downstream concentration and residence time (Reynolds, 1984).

2.1.3 Species selection and algal blooms

Species selection, abundance and dominance is influenced by competitive interactions between algae and herbivorous consumers (Reynolds, 1992). Competition experiments between blue-green algae, green algae and diatoms have shown that blue-green algae can increase to constitute 90 % of the biomass, under extreme light conditions. This dominance occurs even though the blue-greens are initially outnumbered by the other algal groups (Codd and Bell, 1985).

Explanations for this dominance of blue-green algae are the suppression of other phytoplankton by excretion products, and possible protection against grazing by zooplankton by excreting cyanobacterial toxins. Certain blue-green algae are capable of fixing dissolved nitrogen gas, which gives them an advantage over other species of phytoplankton when supplies of combined nitrogen are limiting.

Obviously, species capable of luxury consumption have an advantage over others when nutrient levels fall to limiting levels.

In lakes a clear seasonal succession is often described: diatoms dominate in spring, green algae in early summer, and blue-green algae in summer. In rivers this succession is less clear. On a spatial scale transitions can take place from green algae upstream to diatoms downstream. Successional sequences are generally brief, being subject to abrupt changes in the environment. There is often an evident trend for algae to be more dominant downstream (Reynolds, 1992).

The residence time and discharge of a river will influence the species composition. Parts of the river with high disturbance (i.e. high discharge, and high velocity) favour `ruderal' species, tolerant of high-frequency disturbance. Fast growing opportunists species (`colonists') will take advantage of intervals with less disturbance (declining velocity). In the parts of the river where disturbance is low, species described as stress-strategists may dominate. In the downstream reaches of slow-moving rivers blue-green algae like *Microcystis* may develop and dominate (Reynolds, 1992).

A species will have better prospects for survival if it tolerates lower environmental limits. E.g. nutrient availability (*Anabaena*) or light availability (*Oscillatoria*), and if alternative sources of nutrients can be reached (*Ceratium*, dinoflagellate) (Reynolds, 1982).

Algal blooms (the accumulation of algae at the surface of the water) occur when there is a sufficient supply of nutrients and light, and when the temperature is not limiting. The algal population is further controlled by grazing and sedimentation. In most water systems the nutrients (P and N) are not limiting. Algal growth is thus mainly controlled by the weather, light (intensity and duration) and temperature. Algal blooms especially occur in spring and summer, when light ceases to be the limiting factor (NRA, 1990).

Algal blooms can form and disperse within a matter of hours. They develop most frequently during calm weather. Most reports of algal blooms are from lakes and reservoirs, but high concentrations of algae also occur in rivers (Whitehead and Hornberger, 1981; Beck and Finney, 1987). Blooms are recorded since the Middle Ages. Genera which often are identified as causing algal blooms are: *Microcystis, Anabaena, Oscillatoria, Aphanizomenon* (Reynolds and Walsby, 1975).

Algal blooms have a number of negative aspects. They are an expensive nuisance in water supplies, causing filtration problems. They have an unpleasant odour and taste and in recreational waters spoil fishing and other water sports. Some algal blooms are toxic, and have caused death of fish, birds and cattle. Blue-green algal blooms can lead to extensive and long-lasting alterations in water quality. Periods of complete dissolved oxygen depletion (anoxia) in river bottom waters and sediments can occur when algal blooms die (Lung and Paerl, 1988). This is a major stress factor, and brings the ecosystem out of balance (NRA, 1990; Codd and Bell, 1985; Reynolds, 1980 b).

2.2 MODELLING ALGAE IN RIVERS

2.2.1 Growth factors

A general description of algal growth is given by the expression

$$G = G_{max} * F(L) * F(N) * F(T) * A,$$

in which G is growth, G_{max} is maximum growth rate at 20 °C, F(L,N,T) are limitation factors for light, nutrients and temperature respectively, and A is the algal concentration.

The chlorophyll-a concentration is widely used as a correlative of biomass in estimates of phytoplankton biomass and productivity. Chlorophyll-a is a major photosynthetic pigment, and universally distributed among the photoautotrophic algae. Generally, chlorophyll-a is 0.5 to 2% of the dry-weight (Reynolds, 1984).

Light

Algae need light as a source of energy for their photosynthesis, to transform CO_2 and H_2O in $C_6H_{12}O_6$ and O_2. The light available for photosynthesis depends on the following factors: 1) the amount of light incident to the water surface; 2) penetration of light into the water; and 3) depth of the water column. The interaction between these factors is described by Lambert-Beer's law:

$$I_z = I_0 e^{-\varepsilon z},$$

where ε is the light attenuation coefficient (m^{-1}), I_0 and I_z are the light intensities (photosynthetically active radiation PAR) just below the water surface 0 and at depth z (m) respectively. There is no S.I. unit for solar radiation, commonly used units are μEinsteins.m^{-2}.s^{-1} and W.m^{-2}, other units used are cal.cm^{-2}.s^{-1} and Langley.min^{-1}.

Solar radiation varies seasonally and diurnally, as a function of the changes in the zenith angle of the sun. Incident light is further subject to short-term (e.g. hourly or daily) variation, as a result of natural (unpredictable) changes in cloud cover (Auer and Effler, 1989; Auer and Effler, 1990; James, 1984).

The diminution of light with depth in water differs greatly among rivers and within rivers. The attenuation (or extinction) coefficient is dependent upon several factors, such as suspended solids, humic acids, algae and the background attenuation of the water. A linear equation to describe the dependency of the extinction coefficient on the algal concentration is:

$$\varepsilon = \varepsilon_w + \varepsilon_{chl} * Chl\text{-}a,$$

in which Chl-a is the Chlorophyll-a concentration (μg/l), ε_w is the background extinction coefficient (m^{-1}) and ε_{chl} is the specific algal extinction coefficient ($m^{-1}.(\mu g.l^{-1})^{-1}$).

The relation between solar radiation and algal growth can be described by different formulations. Some formulations take into account light inhibition which causes a reduction in the algal growth rate at light intensities above the optimum light intensity. The most common used equations are Smith's equation, Steele's equation and Monod kinetics.

Smith's equation:

$$p = p_{max} * I * [(I_{0.7})^2 + I^2]^{-1/2},$$

in which p is the instantaneous photosynthesis rate, p_{max} is the light-saturated rate, I = instantaneous light intensity and $I_{0.7}$ is the light intensity at which p = 70% of p_{max} (Bannister, 1974). This equation doesn't describe light inhibition.

Steele's equation:

$$p = p_{max} * (I/I_{opt}) * exp(1 - I/I_{opt}),$$

in which p is the instantaneous photosynthesis rate, p_{max} is the maximum rate of photosynthesis, I is the instantaneous light intensity and I_{opt} is the light intensity for which p = p_{max} (Bannister, 1974). Steele's equation incorporates light inhibition, it describes decreasing algal growth at light intensities above the optimum light intensity.

Monod kinetics:

$$\mu = \mu_{max} * \frac{L}{L + K_l}$$

in which μ is the specific growth rate, μ_{max} is the maximum possible growth rate, L = the light intensity and K_l is the half-saturation value (light intensity for which $\mu = 0.5\ \mu_{max}$).

Because of the diminution of the solar radiation through the water column, it is necessary to integrate the solar radiation over depth to calculate the rate of photosynthesis for the whole water column. Depending on the time step of calculation it can be necessary to integrate over the day as well.

Nutrients

Important nutrients for algae are phosphorus (P), as orthophosphate, and nitrogen (N), as nitrate and ammonium. Most algae prefer ammonium over nitrate as a N-source. Some blue-green algae are capable of fixing N_2-gas as their N-source. In most water systems in the U.K the nutrient concentrations are not limiting. When nutrients are limiting it is usually P first. Silica is an important nutrient for diatoms, as it is used to build their skeleton.

Usually Monod kinetics are used to describe growth when nutrients are limiting, i.e.

$$\mu = \mu_{max} * \frac{N}{N + K_n}$$

in which N is the nutrient concentration, and K_n is the half-saturation constant.

Temperature

Maximum growth rates are dependent on temperature. In general the growth rate increases with increasing temperature, but specific responses vary significantly. A commonly used expression to describe temperature dependency is the Arrhenius expression. This describes a positive relation between growth and temperature with no optimum. From literature it is known that different species have different optimum values for temperature. The Arrhenius expression is useful in describing the average phytoplankton behaviour, and is given by:

$$c_j(T) = c_{j20} D^{T-20},$$

in which $c_j(T)$ is the value of parameter j at temperature T (°C); c_{j20} is the value at 20 °C; and D is a constant. If D = 1.04 it means that the growth increases/decreases by 4% per °C.

2.2.2 Loss factors

In contrast with the growth factors, algal loss is mathematically less well described. Death is usually described as linearly dependent on algal concentration, sometimes dependent on temperature. Sedimentation is usually described as linearly dependent on the sedimentation rate and the depth of the water column. Grazing is usually described as linearly dependent on the predator concentration and the algal concentration.

2.2.3 Dissolved Oxygen and Biochemical Oxygen Demand

Oxygen is produced by algae in their photosynthesis. The production depends on light, temperature, nutrients (if limiting), and the amount of algae. The general relation is:

$$P = y * G,$$

in which y is a yield factor and G is the algal growth (as described in 2.2.1). The yield factor depends on the ratio between carbon and chlorophyll-a in the alga, and the stoichiometry of the photosynthetic reaction.

Most models use a modified, empirical form of this equation. The solar radiation is sometimes expressed as the integrated hours of sunlight. Monod kinetics can also be used to describe photosynthetic oxygen production. Values of photosynthetic oxygen production lie in the range 120-240 mg O_2(mg Chl-a)$^{-1}$day^{-1}.

Respiration (R) depends on the amount of algae, and on the temperature. Rates lie within the range 2.4-48 mg O_2(mg Chl-a)$^{-1}$day^{-1}. The typical variation of R in natural waters falls between 0.04 and 0.1 P_{max} (Reynolds, 1984). Kowalczewski and Lack (1971) derived an empirical relation for the respiration depending on the chlorophyll-a concentration in the River Thames, using dark and light bottle technique.

As algae die they contribute to the BOD. The rate of this contribution is proportional to the death rate of algae.

2.3 DIFFERENT MODELS

Many water quality models have been developed to model algae, both in lakes (or reservoirs) as in rivers. Most models use only the algal concentration to describe DO-BOD relationships. Some models describe the algal growth itself, the influence of solar radiation, and the relations with nutrients, DO and BOD.

Chen (1970) uses in his ecological model Monod kinetics to describe the nutrient limitation. Light limitation is calculated with Lambert-Beer's law. Temperature is not assumed to be a limiting factor.

De Boer (1979) describes a mathematical moving cell model of DO and phytoplankton in rivers. The light intensity is described with the Lambert-Beer expression integrated over depth, and epsilon is linearly related to chlorophyll-a concentration. Growth rate is described with Steele's equation for light, and Monod kinetics for nutrients.

Hornberger and Spear (1980) developed a model to describe benthic algae (*Cladophora*), phytoplankton and phosphorus in a tidal river system. Light is described using the Steele equation integrated over depth and day, with the chlorophyll-a concentration contributing to the extinction coefficient. The influence of nutrients (i.e. P) on the growth rate is described using Monod kinetics. Temperature is linear described.

The QUALL-II model (Câmara and Randall, 1984) describes interactions between DO, BOD, ammonia, nitrite, nitrate, phosphorus, algal biomass, coliforms and radionuclides. Algal growth is described with a growth rate influenced by nutrients using Monod kinetics. Light is described with a modified Monod kinetics.

Bingham *et al.* (1984) use QUALL-II to describe the nitrogen cycle in relation with algal growth in the Great Miami River. Van Benschoten and Walker (1984) also use a modified version of QUALL-II to describe algal growth and nitrogen uptake by algae in the Lower Winooski River.

Young and Saunders (1985) developed a linear model to describe the relation between chlorophyll-a, phosphorus load and flow. With the output of this model, elasticities can be defined, to rank different waste water treatment decisions on their effect on the chlorophyll-a concentration.

Beck and Finney (1987) use a modified form of Monod kinetics, with the instantaneous light intensity calculated using Lambert-Beer's law. It is assumed that algal growth is a function of solar radiation and temperature only. The algae take up nitrogen as ammonium N or nitrate N, and contribute to the balance of DO through photosynthetic oxygen production, and contribute to the BOD load through their mortality.

Qual2e (Brown and Barnwell, 1987) describes interactions between nutrient cycles, algal production, and oxygen cycle. Temperature limitation is described using the Arrhenius

expression. To describe light limitation, several options are available (Smith's function, Steele's equation, half saturation). Nutrient limitation is described using Monod kinetics.

Lung and Paerl (1988) developed a model to describe blue-green bloom effects. With multiple functional groups, a two-layer mass transport and time-variation simulation. The growth rates described with Monod kinetics. Light is described with inhibition at intensities above saturation.

Eutrowasp (Ambrose *et al.*, 1988) describes the relations between algae and nutrients. Temperature limitation is described using the Arrhenius expression. Light limitation is described using Steele's equation integrated over depth. Nutrient limitation is described using Monod kinetics.

Eutrof2 (Aalderink, 1991) describes 3 types of algal species. The interaction between sediment and water column is described. This model is intended for simulation on long time scales. Temperature limitation is described with an optimum curve for each species. Light limitation is described using Steele's equation integrated over depth and day. Nutrient limitation is described using Monod kinetics.

3 Model Development

3.1 QUASAR

The water quality model Quasar (Quality Simulation Along Rivers) has been designed at the Institute of Hydrology to assess the impact of pollutants on river systems. Primary objective of the model is to simulate the dynamic behaviour of flow and water quality along a river system. Forecasting and planning information is generated for key locations along the river.

With Quasar, two options are possible: planning mode and dynamic mode. In the planning or stochastic mode a cumulative frequency curve and distribution histogram of a water quality parameter are generated by repeatedly running the model using different input data selected according to probability distributions defined for each input variable (Monte Carlo simulation). In the dynamic or forecasting mode, the water quality and flow are simulated over selected periods of time.

Flow and nine water quality parameters are modelled: nitrate, ammonia, ammonium ion, dissolved oxygen, biochemical oxygen demand, temperature, E. coli, pH, and a 'conservative' water quality parameter (Whitehead, 1992; Williams, 1993).

Within Quasar a river is divided into a number of reaches. Boundaries of the reaches are chosen at points where major changes in water quality can be expected. Each reach is modelled as a series of well mixed tanks (lags). The model calculates the flow and water quality at the end of each reach. The present version of Quasar makes the assumption that flow is slowly varying. The generalized equation for a water quality variable is thus:

$$\frac{dX}{dt} = \frac{1}{TC}(X_i - X) + \Sigma sources - \Sigma sinks$$

where X_i is the input concentration, X is the output concentration, and TC is the residence time. The equations presently used in Quasar are given in Appendix A. The differential equations are simultaneously solved in a subroutine (Williams, 1993). QSAR is the predecessor of Quasar, it uses the same generalized equations. The algal model is first tested in QSAR, because it is an easier model to make quick changes in.

3.2 DATA SET

There were no sufficient chlorophyll-a data available from the LOIS study area.

Another data set was therefore used, which was available at IH. The set consists of 3 years (1974-1976) of weekly measurements at 6 sites along the Thames: Castle Eaton, Buscot, Swinford, Caversham, Staines and Teddington. These sites form the boundaries of 5 reaches, see Figure 1 (Thames catchment) and Table 1. Measured variables are chlorophyll-a, flow, temperature, and cumulative solar radiation. Plots of chlorophyll-a, flow, temperature and solar radiation are given in Appendix B.

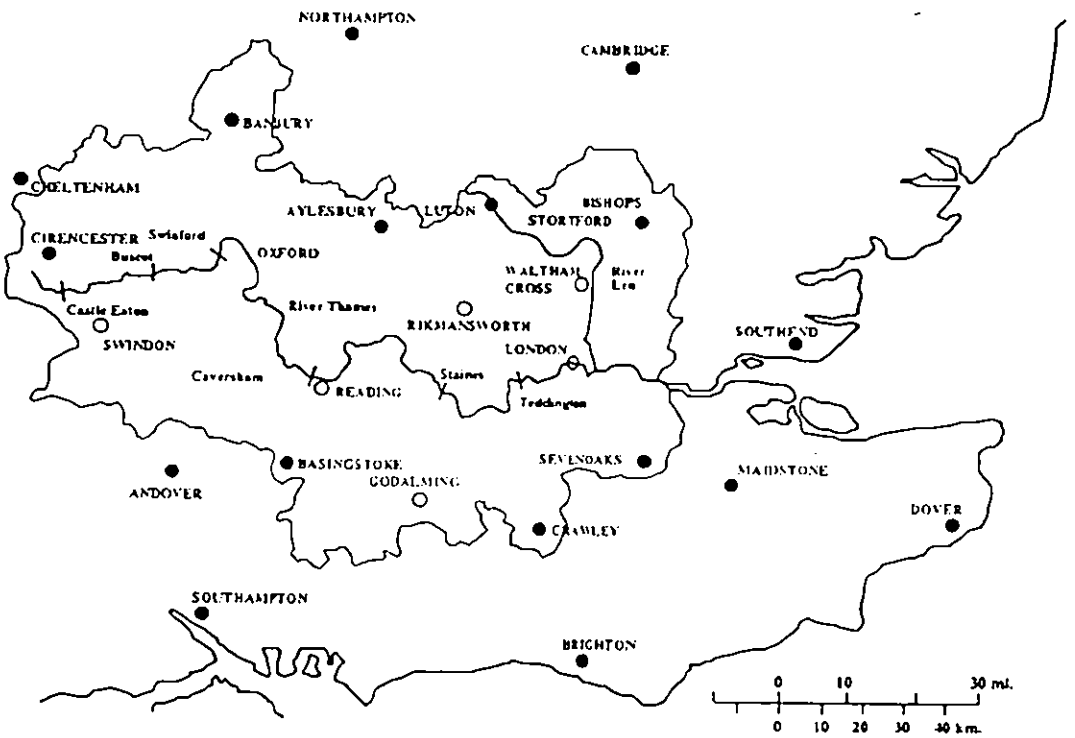

Figure 1: Thames catchment area

There are relatively low levels of chlorophyll-a in the upper reaches of the Thames. Between Swinford and Caversham (reach 3) significant growth occurs. The chlorophyll-a levels downstream show no major increase. Nutrient concentrations in the River Thames are high and unlikely to limit algal growth (Whitehead and Hornberger, 1981; Whitehead *et al.*, 1983; Whitehead and Hornberger, 1984).

Table 1: Chlorophyll-a data 1974-1976

reaches	mean value (µg/l)	max value(µg/l)	reach length (km)
Castle Eaton	10.6	60.2	
Buscot	14.6	113.1	12.8
Swinford	29.1	284.6	32.75
Caversham	57.2	302.1	75.85
Staines	56.9	279.3	55.18
Teddington	61.5	283.5	32.51

3.3 ALGAL MODEL EQUATIONS

The algal model is developed to be a general model to describe chlorophyll-a fluctuations in river systems. It is based on theoretical and empirical relations taken from literature. The described interactions between the major components are given in Figure 2.

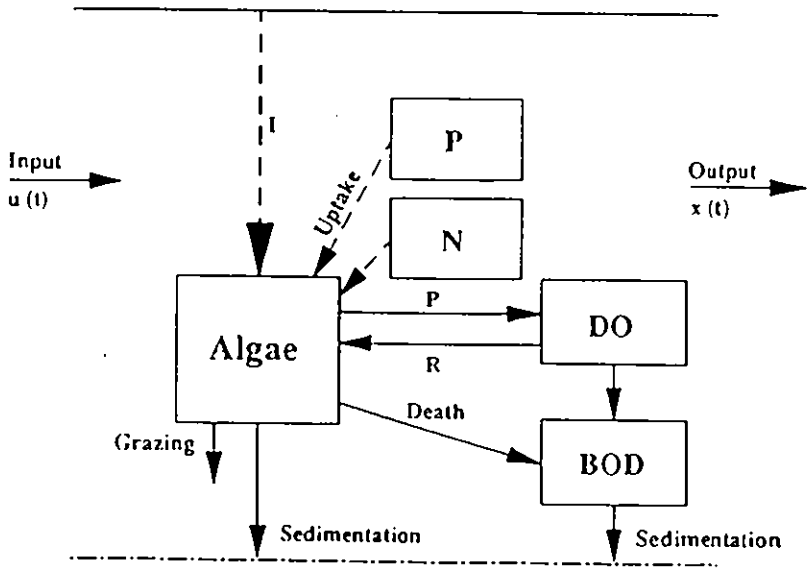

Figure 2: Interactions between the model components

In the model light limitation is calculated with Steele's equation integrated over depth (with Lambert-Beer's Law of attenuation). This equation incorporates inhibition of algal growth above optimum light intensity. The advantage of this equation is that it calculates the light limitation factor using the ratio of observed solar radiation and the optimum solar radiation. The outcome of the calculation is independent on the units in which the solar radiation is given.

Self-shading is defined in the epsilon equation, using a linear relation with the chlorophyll-a concentration. Higher concentrations in chlorophyll-a result in a higher extinction factor.

Temperature limitation is described using the Arrhenius expression, and a base of 1.04. This means that the growth rate decreases/increases by 4% when the temperature changes by 1 °C.

Nutrients are assumed not to be limiting, which is the case in most waters in England. If nutrients are limiting, the relation with the growth coefficient will be described using Monod kinetics.

Loss factors are death and decomposition, grazing and sedimentation. Grazing, death and sedimentation are assumed to be linearly dependent on the algal concentration, and independent on temperature. In the model they are combined as one loss factor.

The change in algal concentration is described using the following differential equation:

$$\frac{dx}{dt} = \frac{u(t) - x(t)}{TC} \qquad \text{(input-output)}$$

$$+ k_1 * F(T) * F(N) * F(L) * x(t) \qquad \text{(growth)}$$

$$- k_2 * x(t) \qquad \text{(death)}$$

$$- k_3 * x(t) \qquad \text{(sedimentation)}$$

$$- k_4 * x(t) \qquad \text{(grazing),}$$

in which: u(t) = upstream Chlorophyll-a concentration ($\mu g.l^{-1}$),

x(t) = downstream Chlorophyll-a concentration ($\mu g.l^{-1}$),

TC = residence time,

k_1 = algal growth rate (d^{-1}),

k_2 = algal death rate (d^{-1}),

k_3 = algal sedimentation rate (d^{-1}),

k_4 = algal grazing rate (d^{-1}),

$$F(T) = 1.04^{T-20},$$

$$F(N) = 1,$$

$$F(L) = \frac{e}{z * \epsilon}\left[e^{-\frac{I_0}{I_{opt}}e^{-\varepsilon z}} - e^{-\frac{I_0}{I_{opt}}}\right]$$

$$\varepsilon = \varepsilon_w + \varepsilon_{chl} * Chl\text{-}a,$$

in which: T = temperature (°C)

I_t = solar radiation at water surface ($W.m^{-2}$),

I_{opt} = optimum solar radiation ($W.m^{-2}$),

z = average depth (m),

ε_w = background extinction coefficient (m^{-1}),

ε_{chl} = algal extinction coefficient (m^{-1} /μg Chl-a.l^{-1}),

Chl-a = chlorophyll-a concentration (μg.l^{-1}),

The growth rate coefficient is for T=20 °C. Loss factors are assumed to be independent on temperature.

Nutrients limitation:

When one of the nutrients is limiting, F(N) is calculated using a Monod kinetics expression,

$$F(N) = \min\left(\frac{N}{N+K_n}\right), \left(\frac{P}{P+K_p}\right)$$

Photosynthetic oxygen production:

The oxygen production is linear dependent on the algal growth. The amount of oxygen produced depends on the μg Chl-a/mg C ratio in the algae, as

$$dO/dt = k_5 * k_1 * F(T) * F(N) * F(L) * x(t),$$

in which: k_5 is the yield factor (mg O_2 per μg Chl-a), which is (32/12)*(mgC/μgChl-a).

Respiration:

The respiration is based on Kowalczewski and Lack's equation (1971), i.e.

$$dO/dt = -(0.14 + 0.013*x(t))*F(T).$$

BOD contribution:

The contribution of algae to the BOD depends on the death rate and the µgChl-a/mgC ratio, i.e.

$$dBOD/dt = k_2*k_5*x(t).$$

Table 2 contains a list of the parameters used in the algal model with suitable ranges of their values.

Table 2: parameter values

	symbol	range
maximum growth rate (d^{-1})	k_1	0.0 - 2.5
death rate (d^{-1})	k_2	0.01 - 0.1
sedimentation rate (d^{-1})	k_3	0.03 - 0.05
grazing (d^{-1})	k_4	0.01-0.10
yield factor O_2 production	k_5	0.03 - 0.09
optimum solar radiation ($W.m^{-2}$)	I_{opt}	5 - 850
background extinction	ε_w	0.3 - 1.3
algal extinction	ε_{chl}	0.016
half-saturation P (µg/l)	K_p	5 - 50
half-saturation N (µg/l)	K_n	1 - 25

The following parameters are set to fixed values, based on a literature survey:

k_5 = 0.0317

BOD contribution = 0.05

ε_{chl} = 0.016

The 3 loss factors (k_2, k_3 and k_4) are combined in 1 parameter (k_{2*}). This results in 4 parameters to calibrate:

k_1 = growth rate

k_{2*} = loss rate

I_{opt} = optimum solar radiation

ε_w = background extinction

In testing and calibrating the model emphasis is given on the ability of the model to describe algal concentration variation, and less on the description of DO and BOD. The Fortran code of the differential equations is given in Appendix C.

3.4 MODEL TESTING

To test the fit of the modelled output with the observed data, a coefficient of determination (R_t^2) is used, i.e.

$$R_t^2 = 1 - \frac{\Sigma e_k^2}{\Sigma (y_k - \bar{y})^2}$$

in which: e_k = observed - model,

y_k = observed,

$\bar{y}$ = mean of observed.

R_t^2 is a normalized measure of the degree of explanation of the data. If e_k^2 is 0, this indicates that the data are modelled perfectly, then R_t^2 has a value of 1. When R_t^2 tends to zero, it indicates that the model has failed completely to explain the data (Young, 1984).

The sensitivity of the model with respect to the parameters is tested by plotting R_t^2 versus one parameter (whilst the other parameters remain constant).

4 Results and discussion

4.1 CALIBRATION AND VALIDATION

Figure 1 (in 3.2) shows the reaches and the major tributaries involved in this study of the River Thames. Using these reaches it was decided that QSAR was not capable of describing the flow conditions adequately from one reach to the next, but that it was capable of describing the flow adequately within a reach. QSAR describes the input from tributaries as a proportion of the incoming river flow only and this can lead to large discrepancies building up progressing down the river network. Also, the water quality of the input tributaries is not described. Each reach is therefore modelled separately, and flow assumed to be constant in each reach. This is a good assumption for reaches 1, 2, 4 and 5, but not for reach 3, where there is a large input from tributaries. Modelling of reach 3 is therefore difficult.

The optimum number of lags for each reach is determined first, with the length of each lag approximately 3 to 5 km. The model is run with a time step of one week, matching the available weekly data. R_t^2 is used to test how well the modelled output describes the observed data, with $R_t^2 = 1$ describing a perfect fit. The parameter set with the best fit is found by an educated trial and error procedure. Each parameter is optimized separately, with the best parameter values then optimized together. Limits for the variation of each parameter are set a priori.

The reaches are calibrated with the data of 1974. Results of these calibrations are given in Table 3 and Figures 3 to 7.

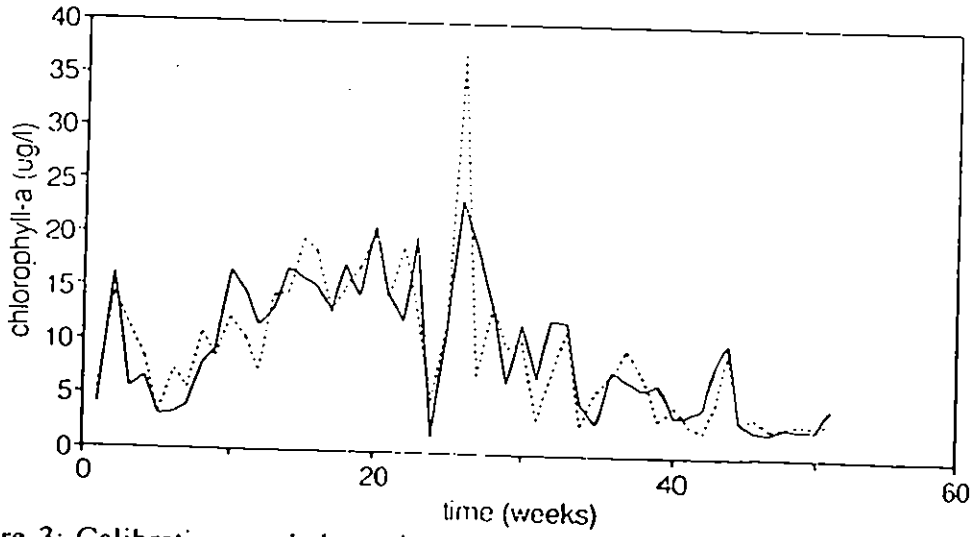

Figure 3: Calibration reach 1; ··· observed - model

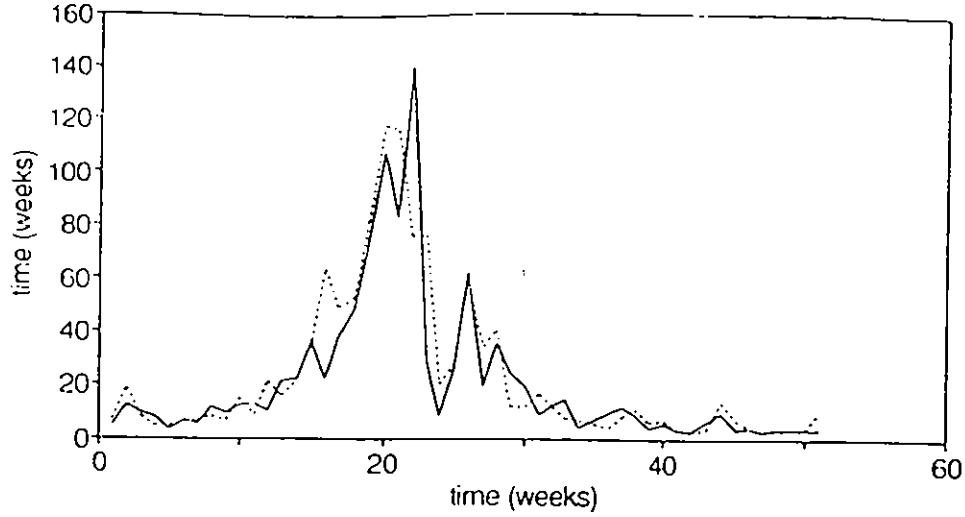

Figure 4: Calibration reach 2; ··· observed - model

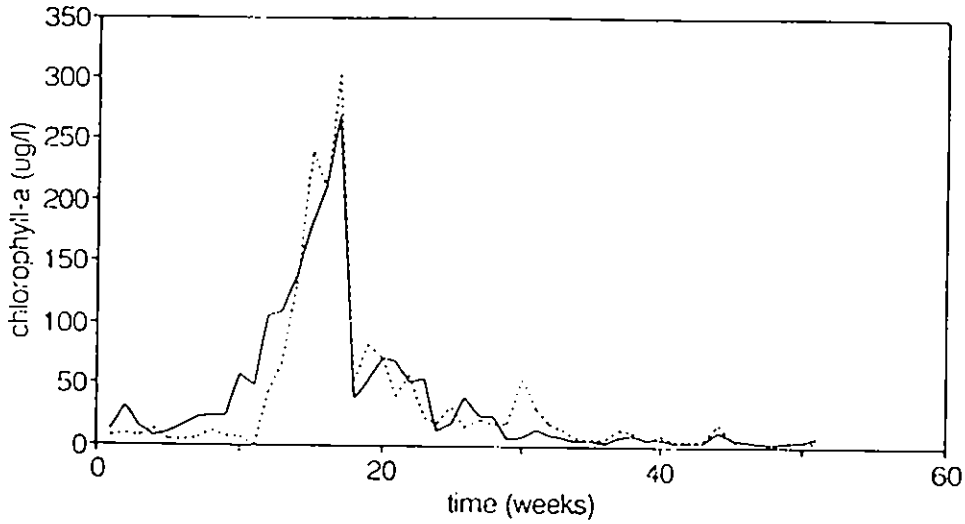

Figure 5: Calibration reach 3; ··· observed - model

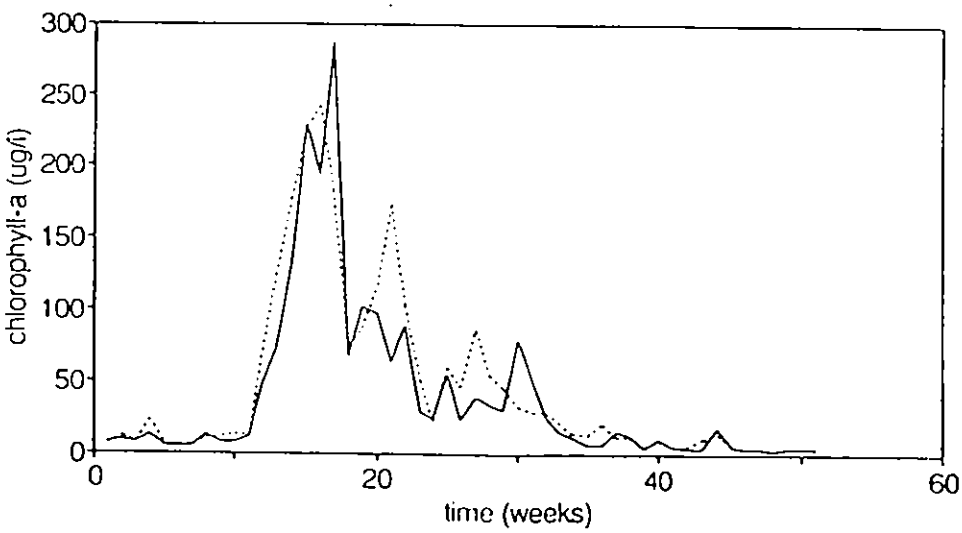

Figure 6: Calibration reach 4; ··· observed - model

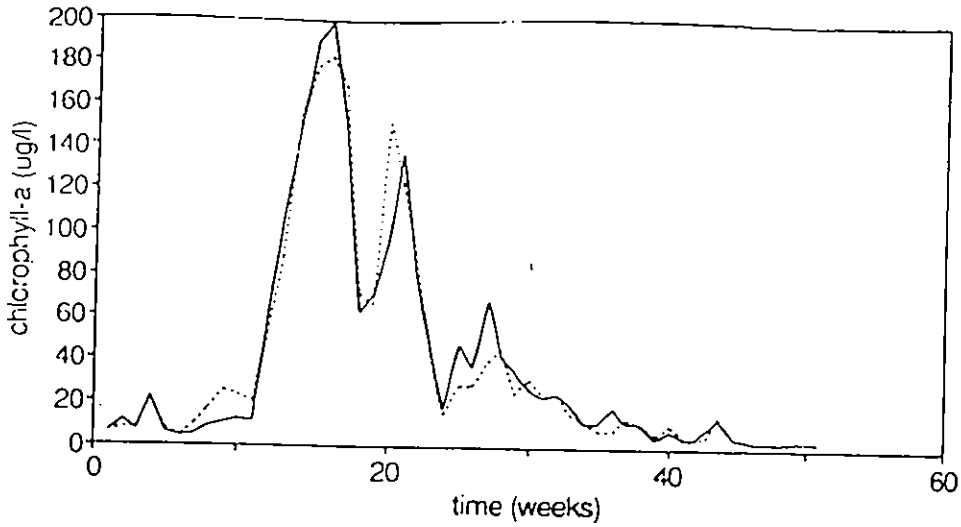

Figure 7: Calibration reach 5; ··· observed - model

Table 3: Calibrated parameters and R_t^2 for each reach using 1974 data.

	reach 1 Buscot	reach 2 Swinford		reach 3 Caversham		reach 4 Staines	reach 5 Teddington
length (km)	12.8	32.75		75.85		55.18	32.51
no. of lags	4	10		18		10	8
k_1 (week^{-1})	1.3	(8)	1.3	(9)	1.5	3.5	1.3
k_2. (week^{-1})	0.15	(1.2)	0.10	(1.2)	1.2	0.9	2.5
ε_w (m^{-1})	2.0	(0.75)	0.80	(0.80)	0.80	0.2	0.7
I_{opt} (W.cm^{-2}.w^{-1})	5000	(40000)	10000	(5000)	5000	16000	3000
R_t^2	0.653	0.739		0.871		0.789	0.945

Reaches 2 and 3 proved to be difficult to calibrate with only one parameter set. This problem is solved by describing the spring bloom with one set of parameters (given between parentheses), and the remaining period with a second parameter set. In this way the algal concentration throughout the whole period can be modelled well, and it identifies the fact that spring blooms behave differently compared to summer blooms.

Reach 1 (Figure 3) is modelled quite well. The peaks are timed well, one peak is underestimated. Reach 2 (Figure 4) is described well using 2 parameter sets. The spring

bloom is timed well, but slightly overestimated. Reach 3 (Figure 5) is difficult to model. The spring bloom is timed well, but slightly underestimated. Reach 4 (Figure 6) is modelled reasonably well. The timing of the blooms is good. The model slightly overestimates the spring bloom, and underestimates the early summer bloom. Reach 5 is modelled well. The spring and early summer blooms are timed well, the concentrations are modelled correctly.

The parameter sets are validated with the data of 1975 and 1976, R_t^2 values for both years are given in Table 4. The validation plots for 1975 are given in Figures 8 to 12. The conditions in 1975 are similar to 1974; similar flow, solar radiation and temperature. R_t^2 values are low, except for reach 5. High values of e_k^2 (causing low values of R_t^2) are sometimes caused by only a few points with a big error, see Figure 13.

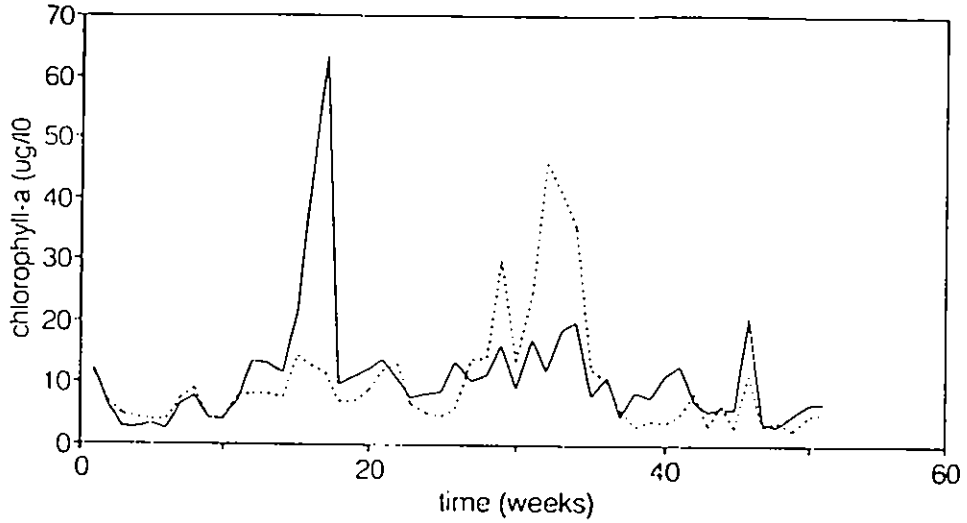

Figure 8: Validation reach 1 1975; ··· observed - model

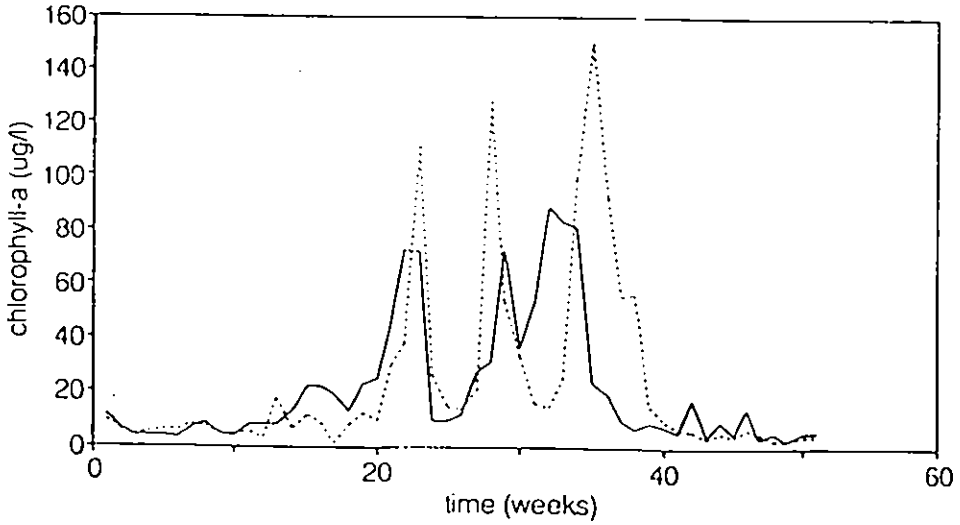

Figure 9: Validation reach 2 1975; ··· observed - model

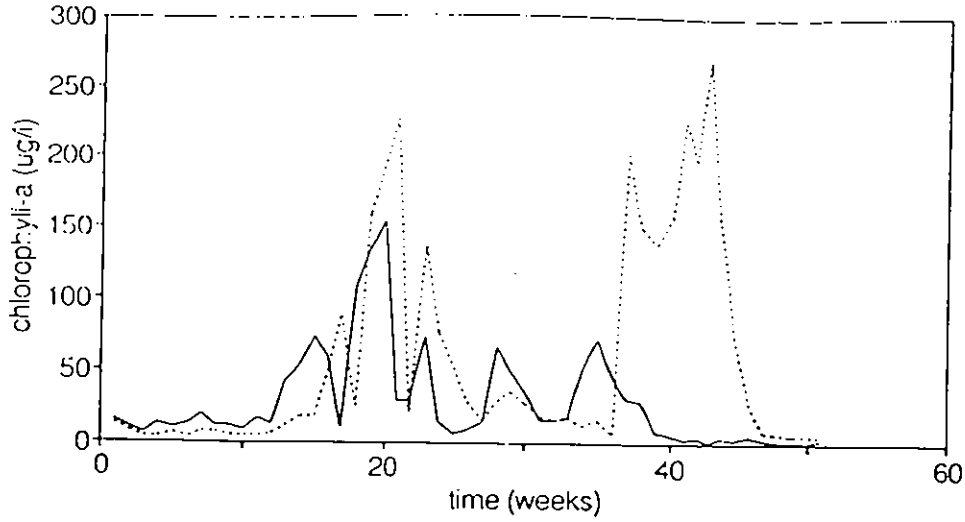

Figure 10: Validation reach 3 1975; ··· observed - model

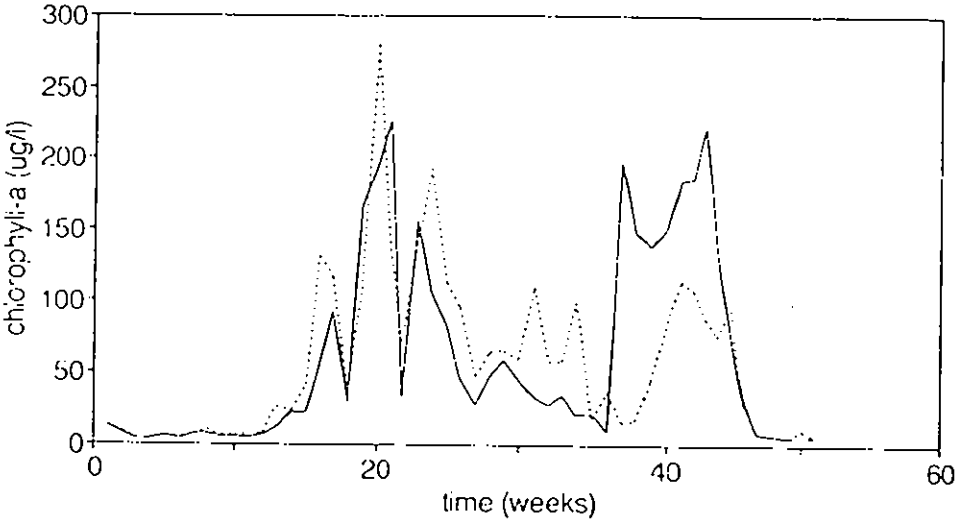

Figure 11: Validation reach 4 1975; ··· observed - model

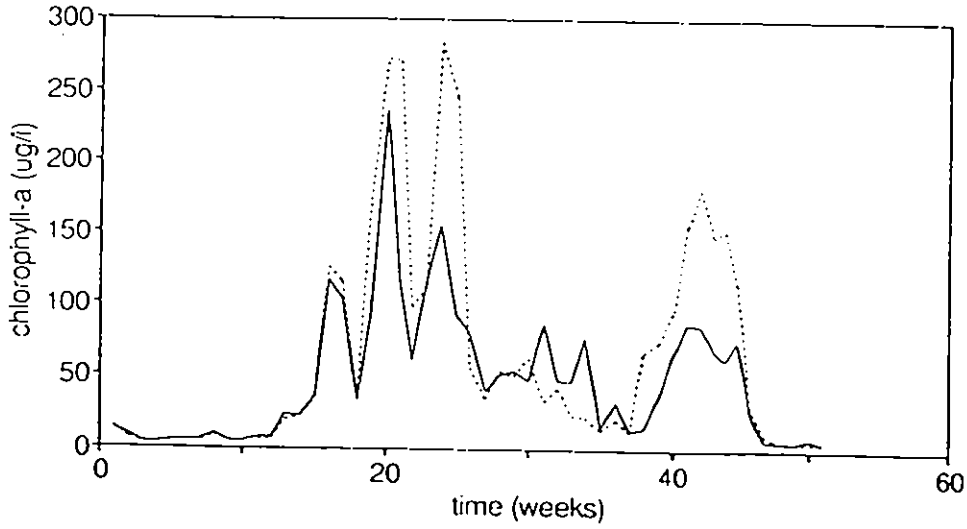

Figure 12: Validation reach 5 1975; ··· observed - model

Table 4: R_t^2 of validation for 1975 and 1976

	reach 1	reach 2	reach 3	reach 4	reach 5
1975	-0.419	0.128	-0.238	0.075	0.621
1976	0.310	-2.130	-0.735	0.157	0.420

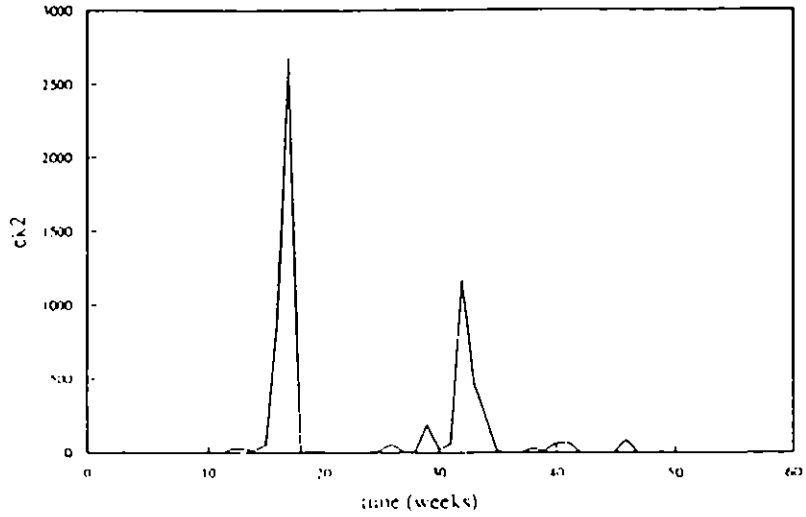

Figure 13: Peaks of e_t^2 determining R_t^2, for reach 1, 1975

The validation of reach 1 (Figure 8) shows large differences in modelled and observed concentration, the timing of the peaks however is reasonable. In reach 2 (Figure 9) the timing of the spring and early summer bloom is correct, but the summer bloom is predicted too early. The concentration of all three peaks is underestimated. The late summer bloom in reach 3 (Figure 10) is not modelled. The spring blooms are timed slightly too early, and the concentrations are underestimated. In reach 4 (Figure 11) the timing of the blooms are correct, but the spring bloom concentration is underestimated, and the late summer bloom overestimated. In reach 5 (Figure 12) the spring blooms and the late summer bloom are timed well. The concentrations of the blooms are slightly underestimated.

1976 was a year with extreme conditions; with low flows, high temperatures and high solar radiation values during the summer. Major blooms of *Microcystis* occurred (Whitehead and Hornberger, 1981). Validation for 1976 is more difficult, because of these extreme conditions. Validation plots for 1976 are given in Appendix D. For most reaches the timing of the peaks is reasonable, but the concentrations are not predicted well, peaks are either underestimated or overestimated. Validation of reach 3 with 1976 is particular problematic,

this is caused by the combination of extreme conditions and the inadequacy of QSAR to describe input from tributaries. This reach is therefore also calibrated for 1976. Using two parameter sets it is possible to model this reach for 1976. The plot is given in Appendix E.

4.2 SENSITIVITY OF THE MODEL

The sensitivity of the model for the parameters is tested using 3 reaches, an upstream reach (1), a middle reach (3) and a downstream reach (5). The variation in R_t^2 is calculated for a range of values for one parameter, with the other three parameters constant. Results are given in Table 5. Plots of R_t^2 for reach 3 are given in Figures 14 to 17.

Table 5: R_t^2 sensitivity

parameter range	reach 1	reach 3	reach 5
k_1 (0 to 10.0)	-200 to 0.654	-0.4 to 0.531	0.840 to 0.945
k_2. (0 to 4.0)	-0.5 to 0.641	-2.3 to 0.531	0.827 to 0.945
ε_w (0 to 3.0)	0.580 to 0.654	0.487 to 0.575	0.944 to 0.945
I_{opt} (100 to 50000)	0.537 to 0.654	0.135 to 0.633	0.944 to 0.945

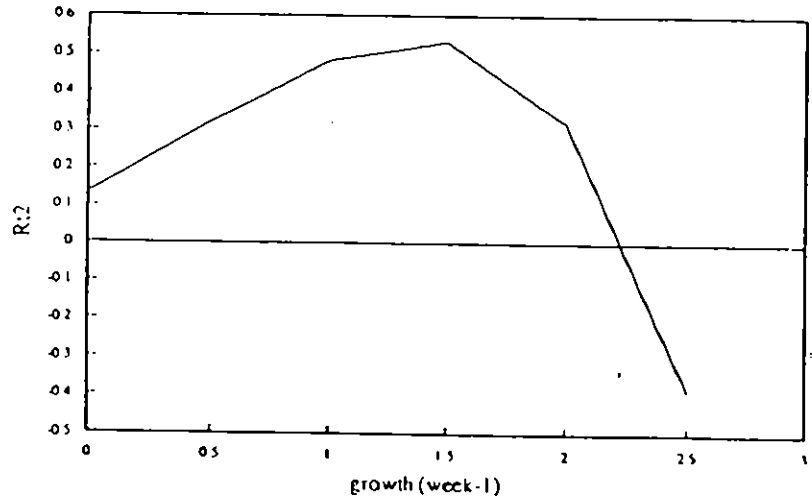

Figure 14: Sensitivity for k_1

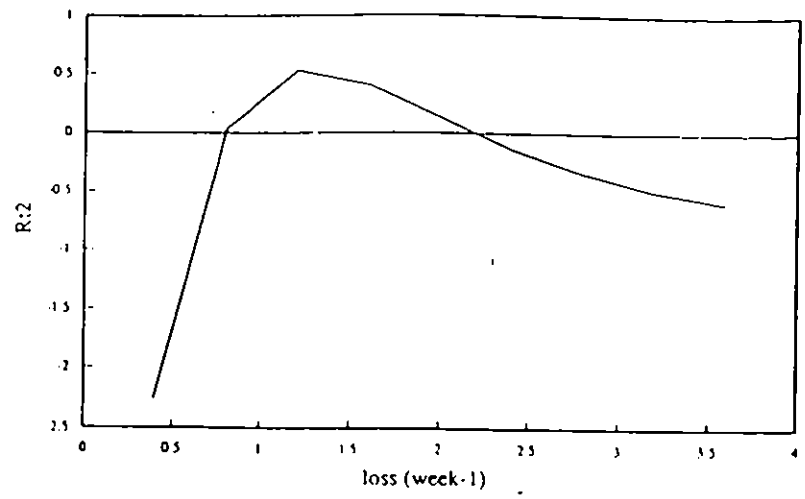

Figure 15: Sensitivity for k_2.

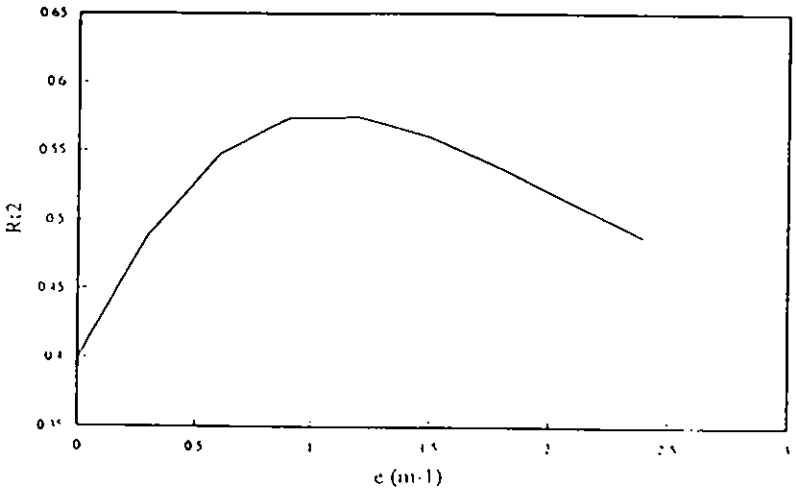

Figure 16: Sensitivity for ε_w

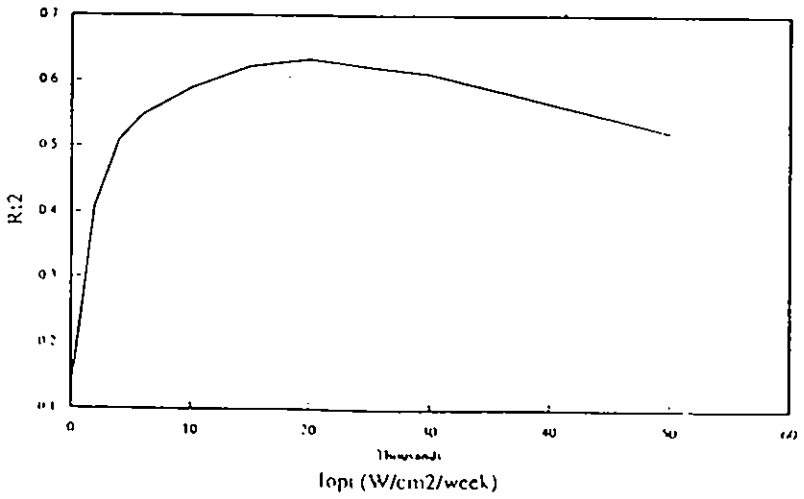

Figure 17: Sensitivity for I_{opt}

The model is highly sensitive to the growth (k_1) and loss parameter (k_2.), a small change in these parameters can cause a large change in R_1^2. The growth and loss parameter have a direct influence on the chlorophyll-a concentration. The model is less sensitive to I_{opt}, and least sensitive to ε_w. The last two parameters have an indirect influence on the chlorophyll-a concentration, since they form part of the light limitation factor F(L). Figure 18 shows the effect of ε_w on F(L) for different values of I_{opt} and an average value of 16000 ($W.cm^{-2}.w^{-1}$) for I_t and an average value of 40 ($\mu g.l^{-1}$) for the chlorophyll-a concentration. It shows that the value of ε_w for the maximum F(L) factor decreases with increasing I_{opt}. ε_w and I_{opt} combined determine the value of the F(L) factor.

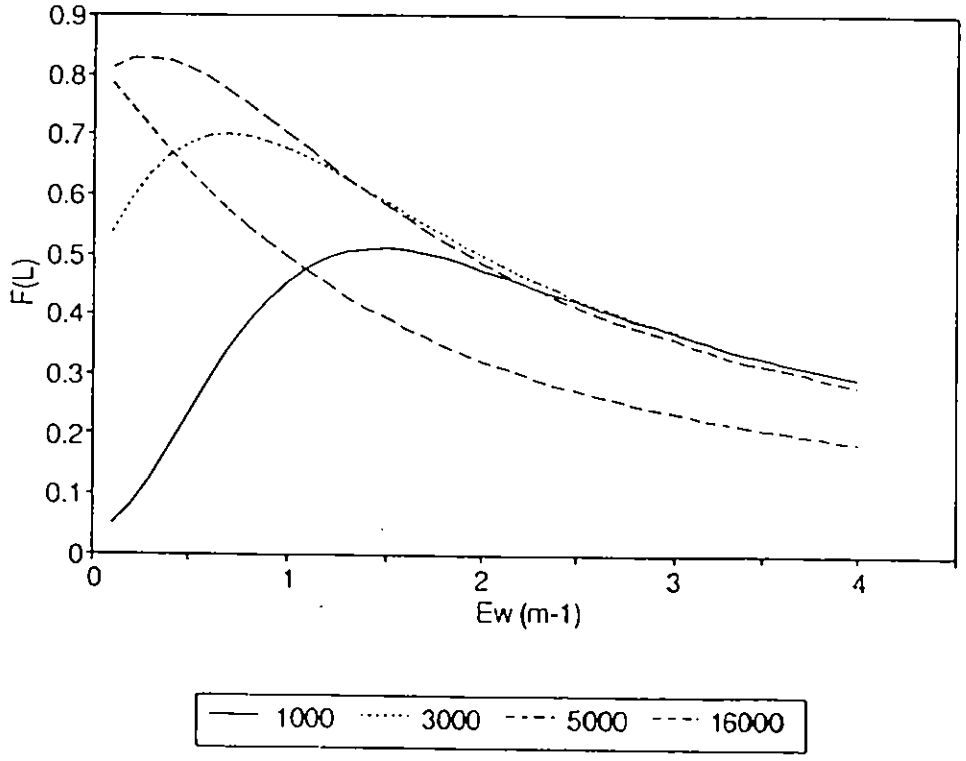

Figure 18: F(L) versus ε_w at different I_{opt}

The sensitivity of the model to the parameters also depends on the reach. Reaches 1 and 3 are much more sensitive than reach 5. Reach 1 is a stable reach, with little algal growth, whereas reaches 2 and 3 are more dynamic, with significant algal growth and an

increase in flow. Reaches 4 and 5 are stable again, with little growth and steady flow. In reach 5 the algal concentration is mainly determined by the input conditions, and is less sensitive to changes in the parameters.

4.3 DISCUSSION

Chlorophyll-a concentrations in reaches 1, 4 and 5 are well described using the model. Reaches 2 and 3 are difficult to describe using only one parameter set, but are well described using two parameter sets. Reach 3 in particular is difficult to model, which can be explained by the length of the reach, and the increase in flow caused by input from tributaries. The quantity and quality of this input is not represented in the model, whereas it could change the water quality of the reach.

The results of the validation of the parameter sets depend on the reach and the year. The results are not as good as the calibration, because of the different environmental conditions and algal behaviour in each year. The model predicts chlorophyll-a concentrations, and cannot distinguish between different algal species. This presents a problem since in another year, other algal species with different behaviour can dominate.

The model is able to describe chlorophyll-a fluctuations in rivers. Some peaks are under- or overestimated. Upstream conditions are mainly responsible for the timing of the peaks. The parameters have mainly an influence on concentration of the peaks. The flow and residence time are important factors controlling algal populations in river systems.

Strong and weak points of the model:

The model gives a good estimation of algal concentrations and timing of peaks. It can be used as a predictive tool in water quality management. It is a simple model, with 4 parameters and is therefore easy to calibrate. When it becomes part of Quasar, it will have only 3 parameters.

The simplicity of the model is at the same time a weak point. It describes chlorophyll-a and makes no distinction between different algal groups. This weakness is shown by the difficulties in calibrating reach 2 and 3, and validating with the 1976 data set. The solution to this problem is to calibrate the spring bloom separately, as if modelling two different algal species.

There is no detailed relationship with the nutrient cycles in this model. The assumption that nutrients are not limiting is valid for the Thames, but when the water quality improves nutrients can become limiting. Nutrient limitation will be described in Quasar.

Biological meaning of the parameter values:

The values of k_1 correspond well with reality. There is little growth in reach 1 (k_1=1.3 $week^{-1}$). The main growth occurs in reaches 2 and 3 (k_1=8 and 9 respectively in spring). Reaches 4 and 5 have less growth again (k_1=3.5 and 1.3 respectively). From the literature a wide range of growth values is known, from 3.2 ($week^{-1}$) to 20 ($week^{-1}$) (Moss, 1980; Reynolds, 1984).

The loss parameter (k_2) is low in reach 1, reaches 2 and 3 have a higher value. These reaches are more dynamic. Reach 5 has quite a high loss factor, but as shown in Table 5 this reach is not very sensitive to the loss factor.

I_{opt} varies in a wide range. From the literature a wide range of different values are known as well. The high value in reach 2 of 40000 ($W.cm^{-2}.week^{-1}$, ≡ 661 $W.m^{-2}$) has little biological meaning. The values in reaches 1, 3 and 5 of 5000 and 3000 ($W.cm^{-2}.week^{-1}$) (≡ 83 and 50 $W.m^{-2}$ respectively) have more biological meaning. The value in reach 4 of 16000 ($W.cm^{-2}.week^{-1}$, ≡ 265 $W.m^{-2}$) is rather high. Reynolds (1984) gives values for I_{opt} ranging from 5 to 73 $W.m^{-2}$. Other models have values for I_{opt} ranging from 70 to 250 ($W.m^{-2}$) (Hornberger and Spear, 1980), and around 150 ($W.m^{-2}$) (Lung and Paerl, 1988). Despite the less biological meaning of the values for I_{opt} in this model, the parameter performs an important role in the model as a 'fudge factor', in making the model describe the observed data. The model is reasonable sensitive to I_{opt}.

ε_w has a range of values. In reach 1 (with little growth) it has a value of 2 (m^{-1}). In the reaches 2, 3 and 5 it has a lower value of around 0.8 (m^{-1}). The value in reach 4 is very low; 0.2 (m^{-1}), this corresponds with an unrealistic high clarity of 1.50 (m). The model is the least sensitive to this parameter.

The parameter sets as a whole reflect the biological processes. In each reach the individual parameters vary in biological meaning. The growth and loss parameter have meaningful values, but the values of I_{opt} are less meaningful. ε_w is meaningful but the model is not very sensitive to this parameter.

Differences between reaches:

The calibration of the model with separate reaches has resulted in different parameter values for each reach. This spatial variability can be explained by the differences in residence time for each reach. The residence times for the summer period (June-September) are given in Table 6; calculated using the mean width, depth, length and average summer (low) flow for each reach.

Reach 3 has the longest residence time, in this reach the situation is favourable for rapid growth of colonists species and stress-tolerant species. The residence time in the other reaches is shorter, and decreases downstream. The residence time increased more than twofold

in 1976, this combined with the high temperature and solar radiation created a situation ideal for a blue-green (*Microcystis*) bloom.

Table 6: Average summer flow residence time for each reach

	1974		1975		1976	
reach	days	days/km	days	days/km	days	days/km
1	1.769	0.138	4.758	0.372	10.302	0.805
2	3.329	0.102	7.054	0.216	21.421	0.654
3	25.808	0.340	59.145	0.780	120.69	1.591
4	4.154	0.075	7.134	0.129	13.535	0.245
5	1.862	0.057	3.199	0.098	5.621	0.173

Comparison with other models:

With the QSAR algal model, the same accuracy in results is achieved as with the Thames algal model developed by Whitehead and Hornberger (1984), based on the same data set.

The description of the algal growth is basically the same as in the models Qual2e (Brown and Barnwell, 1987), Eutrowasp (Ambrose *et al.*, 1988) and Eutrof (Aalderink, 1991). Nutrient limitation is not described in the current version for QSAR, but will be in Quasar. Eutrof and Eutrowasp are specific eutrophication models, and have a detailed description of the interactions with the nitrogen and phosphorus cycle.

Beck and Finney (1987) in their research find spatial variability in algal behaviour in upstream and downstream parts of the river. This corresponds with the different parameter values for the reaches in this model.

Van Benschoten and Walker (1984) find that when algae are controlling the system, the use of a steady-state model is difficult because important environmental changes result from unsteady-state processes, i.e. there are daily variations in photosynthesis and sudden die-off of algal blooms. Quasar is a dynamic model, it can describe the daily variation in photosynthesis (depending on the time step of calculation). The sudden die-off of algal blooms is an unpredictable event and difficult to describe with a steady-state model.

Lung and Paerl (1988) find that the river flow is one of the key factors determining the establishment and maintenance of a blue-green algal bloom. Blue-green (*Microcystis*)

blooms especially occur with low flow and warmer than usual temperatures. This corresponds with the situation of 1976 in the Thames, with low flows and warmer temperatures causing a *Microcystis* bloom.

5 Conclusions and recommendations

With the algal model part of an integrated water quality model, good predictions of the chlorophyll-a concentrations in the River Thames can be attained. The algal model is a general model, and is therefore not aimed to be the most detailed algal model possible. Neither is it a specific eutrophication model. Phytoplankton is described as chlorophyll-a, with no distinction made between different algal groups. The parameters describe average algal behaviour. Diatoms and blue-green algae for example are assumed to behave similar.

Ecological (food web) structures are difficult to describe mathematically. Before one starts to model (a part of) this ecological web, it is important that one understands the ecology behind the equations. This is a model, a simplification of reality. The output is an estimate, a prediction of chlorophyll-a concentrations.

It is recommended that the same set of algal equations used in QSAR should be incorporated in Quasar, with additional modifications. The modified equations for Quasar are given in Appendix F, with the additional modifications mentioned as follows.

- The background extinction (ε_w) set to a fixed value of 0.8 (m^{-1}). This value is based on the calibration results in this model and values known from literature (Hornberger and Spear, 1980; Reynolds, 1984).

- An average ratio of 30 µg Chl-a/mg C, used in the DO and BOD equations.

- The loss factor split into sedimentation, grazing and death. Sedimentation is dependent on depth, and described with a fixed value of 0.10 ($m.d^{-1}$), this can be linked with the benthic oxygen demand. Grazing is described with a fixed value of 0.05 (d^{-1}). The death rate is described with a parameter to calibrate, linked with BOD.

- A threshold value of 8 °C below which the growth rate is zero.

- Nutrient limitation described with Monod kinetics, if the nutrient concentrations are below threshold values.

If the flow for a river is modelled well in Quasar, the algal model is capable of describing algal fluctuations. The flow and residence time are important factors controlling

algal populations in rivers. Needed as input for the model are the upstream and boundary conditions (flow, and chlorophyll-a concentration), and solar radiation and temperature. The algal model can be used as a predictive tool in water quality management.

It is important that the limiting factors for algal growth are well described. A weak point in Quasar at the moment is the light (solar radiation) description. The solar radiation is a constant value for the whole day, assuming 4 hours sunlight per day. The length of the daylight period is determined from longitude and latitude data and the time of year.

Temperature is modelled as a conservative variable in Quasar, assuming that heat exchange at the surface is negligible.

Nitrate and ammonia are modelled in Quasar, and will be linked to the algal model. In most systems phosphate is the first limiting nutrient for algal growth. A phosphate model therefore needs to be developed for Quasar.

Aspects for further research:

- Calculation of solar radiation. The present calculations in Quasar are very basic, and leave room for improvement. Possibility is to calculate the light pattern as a semi-sinusoidal curve. This can be combined with a data set for hours of sunlight for each day/month, to simulate seasonal variation in cloud cover.

- Nutrients are described with Monod kinetics. This is how most models describe nutrient limitation. Nutrient kinetics in reality are more complicated than this description. The nutrient concentration in the water is not necessarily the available concentration for the alga. Fluxes and the content in the algal cells, and the nutrient interactions with sediment are not included. Luxury consumption, when algae take up more nutrients than necessary, is difficult to describe. It enables algae to continue to grow when nutrient levels fall below limiting concentrations.

- Succession and dynamics of the composition of the algal population can be simulated by three sets of algal equations, describing diatoms, green algae and blue-green algae separately. For calibration specific algal data are needed.

- Loss by death and grazing is described with a linear relation to algal concentration only. In reality, respiration is also dependent on temperature. And grazing is a much more complicated mathematical problem since the food web has to be described. It partly depends on the predator concentration (zooplankton), the filtering rate of the

predators, and the preferences of the predators.

- Extinction caused by turbulence and resuspension can be a factor of influence in some rivers. This can possibly be described in the epsilon equation by making ε_w depend on the flow.

- The dependency of epsilon on chlorophyll-a is described with a linear relation. Another possibility is a non-linear dependency, as used in Qual2e (Brown and Barnwell, 1987),
  $\varepsilon=\varepsilon_{chl1}$*Chl-a + ε_{chl2}*Chl-$a^{2/3}$.
  To test which relation describes the dependency of epsilon best, research on a data set with observed chlorophyll-a concentration and extinction is needed.

- Prediction of the effect of climate change, i.e. lower flow and higher temperature, on the chlorophyll-a concentration in the River Thames.

- Validation of the parameters proved to be difficult. Calibration of the model with the 1975 and 1976 data sets will be useful, and give extra insight in the variation in algal population from year to year.

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Appendix A

Differential Equations Quasar

Flow, only needs to be solved for the case when C is not 1:

XP(1)=(U(1)-XO(1))/TCC

Conservative:

XP(3)=(U(3)-XO(3))/TC

Temperature:

XP(7)=(U(7)-XO(7))/TC

Dissolved Oxygen:

XP(4)=(U(4)-XO(4)+WEIR2)/TC

+K11	Algae O_2 contribution
-K4*K6*XO(4)	Sediment respiration
+K2*(CS-XO(4))	Reaeration
-K15*4.57*XO(6)	Ammonia O_2 demand
-K1*XO(5)	O_2 loss from BOD

Nitrate:

XP(2)=(U(2)-XO(2))/TC

-K5*XO(2)

+K15*XO(6)

Biochemical Oxygen Demand:

XP(5)=(U(5)-XO(5))/TC

-K1*XO(5)	
+K10	BOD contribution by algae
-K18*XO(5)	loss of BOD by sedimentation

Ammonia:

XP(6)=(U(6)-XO(6))/TC

-K15*XO(6)

E. coli:

XP(8)=(U(8)-XO(8))/TC

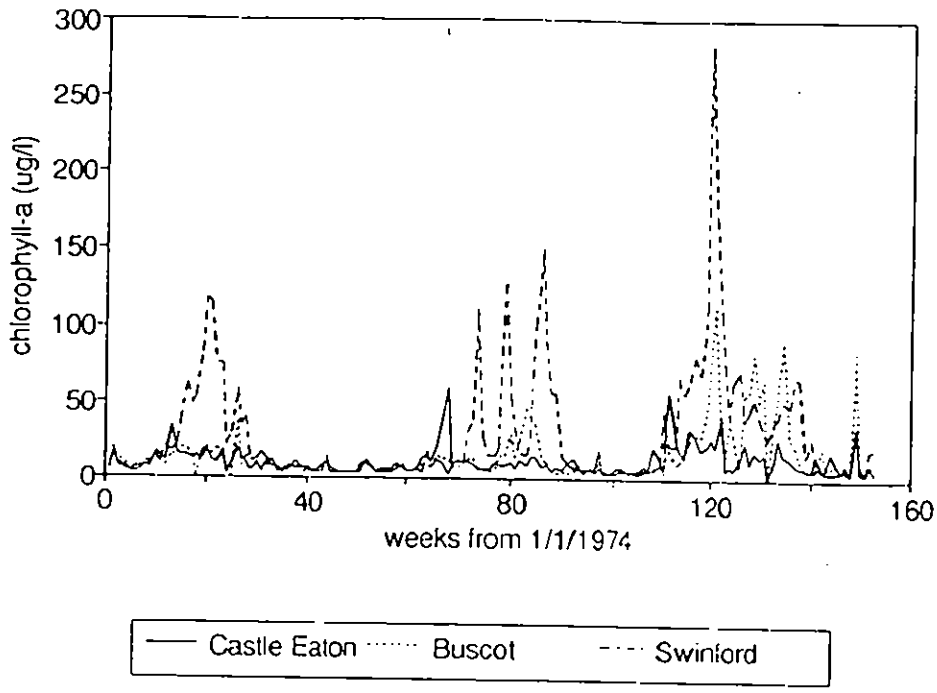
-K16*XO(8)	Rate of decay of E coli
+K19*XO(8)	Rate of resuspension of E coli

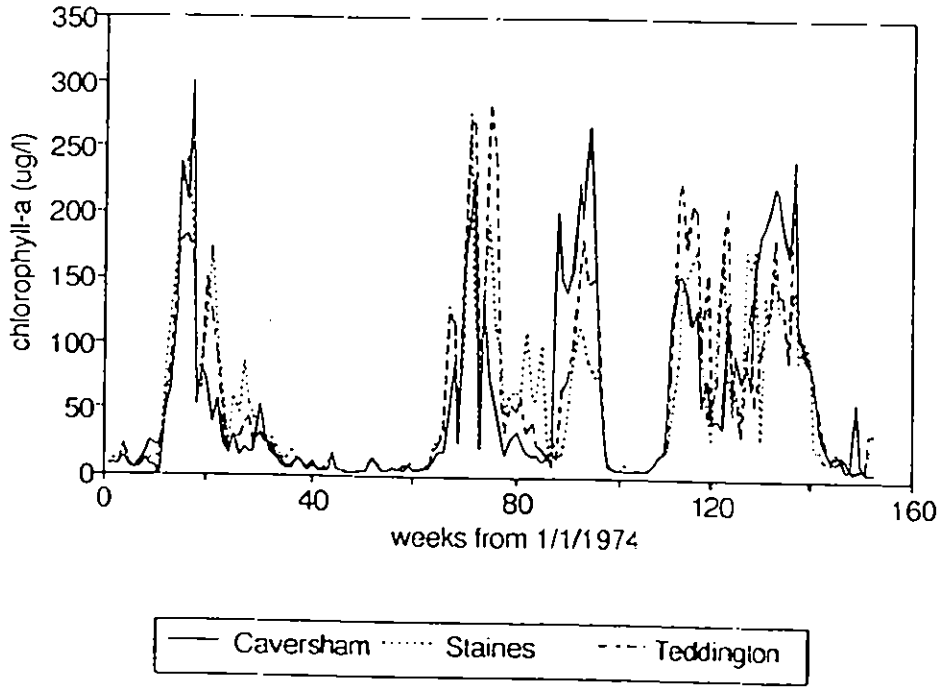
pH:

XP(9)=(U(9)-XO(9))/TC

Appendix B

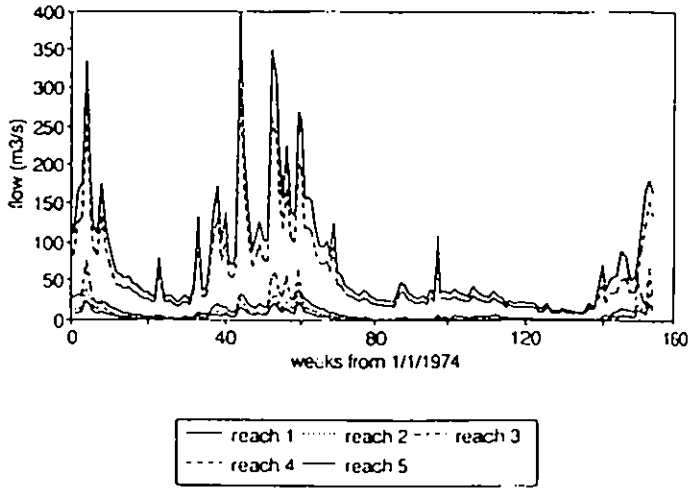
Data set



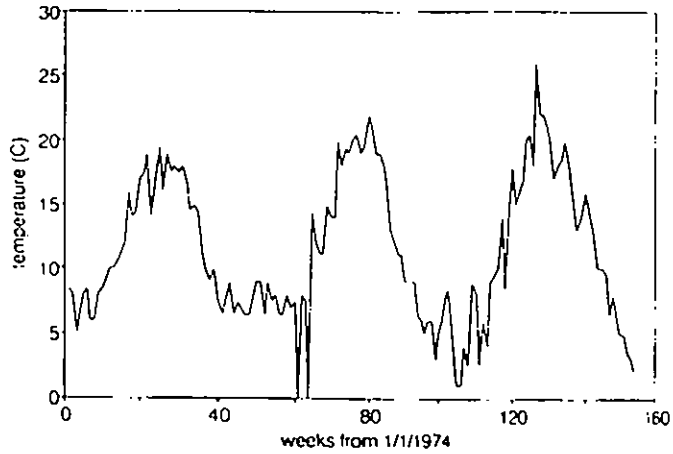


Chlorophyll-a concentrations 1974-1976

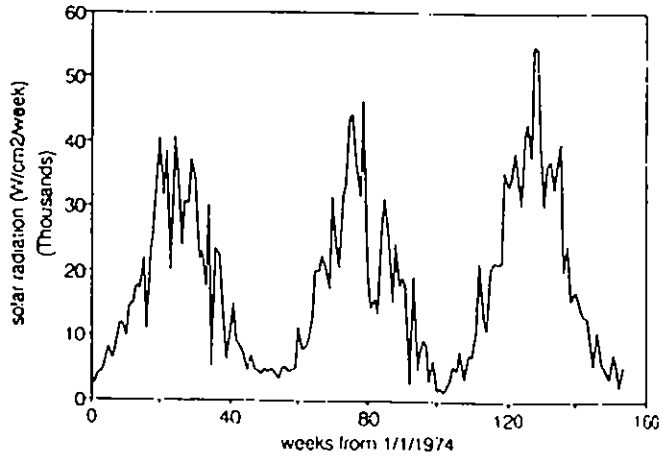
Appendix B



Flow 1974-1976



Temperature 1974-1976



Solar radiation 1974-1976

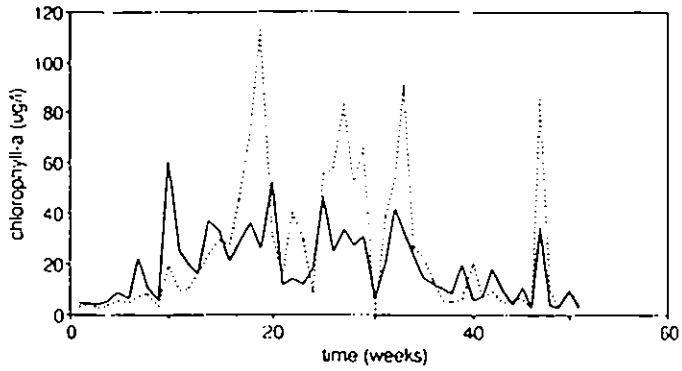
Appendix C

QSAR Fortran code

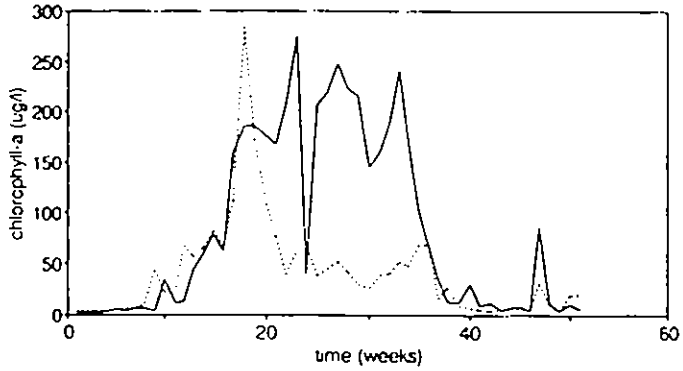
```
      SUBROUTINE DEQN(XO,T,N,XP,TPD,SOLRD,IKTD)
C
C THIS ROUTINE DEFINES THE D.E. FOR THE RIVER FLOW MODEL.
C THE EQUATION IS BASED ON MASS BALANCE EQUATIONS.
C THIS ROUTINE IS USED WHEN AN IMPULSE IS PUT INTO THE RIVER.
C
      REAL XP(7),XO(7)
      REAL TPD(153),SOLRD(153)
      COMMON /DE/ U(7),TC,C1,C2,C3,C4,C5,C6,C7,C8,C9,
     1           C10,C11,P1,P2,P3,P4,ITH
      COMMON /DEQ/ CC1,CC2,CC3,CC4,CC5,CC6,CC7,CC8,
                   CC9,CC10,CC11,H
      COMMON /CCFILE/ IPFF,IPFP,IOP,IIP
C
      CS =14.541233-0.3928026*TPD(IKTD)+0.00732326*(TPD(IKTD)**2)-
     1    0.00006629*(TPD(IKTD)**3)
      TEMP = 1.04**(TPD(IKTD)-20.)
      EPS = CC10+0.016*XO(7)
      RI=(2.718/(2.*EPS))*(EXP((-SOLRD(IKTD)/CC9)*EXP(-2.*EPS))-
     1    EXP(-SOLRD(IKTD)/CC9))
C
C XP(1) IS FLOW.
      XP(1)=(U(1)+P4)/TC -XO(1)/TC
C XP(2) IS CONSERVATIVE.
      XP(2)=(U(2)+P1)/TC-XO(2)/TC
C XP(3) IS E COLI
      XP(3)=(U(3)+P2)/TC-XO(3)/TC-CC2*TEMP*XO(3)
C XP(4) IS NITRATE.
      XP(4)=(U(4)-XO(4))/TC-CC4*TEMP*XO(4)
C XP(5) IS DISSOLVED OXYGEN.
         XP(5)=(U(5)-XO(5))/TC+CC5*(CS-XO(5))
        -CC6*TEMP*XO(6)+0.0317*CC8*TEMP*RI*XO(7)-(0.14+0.013*XO(7))*TEMP
C XP(6) IS B.O.D.
        XP(6)=(U(6)+P3)/TC-XO(6)/TC-CC6*TEMP*XO(6)-CC7*XO(6)+0.05*XO(7)
C XP(7) IS ALGAE
      XP(7)=(U(7)-XO(7))/TC+CC8*TEMP*RI*XO(7)-CC11*XO(7)
      RETURN
      END
```

Appendix D

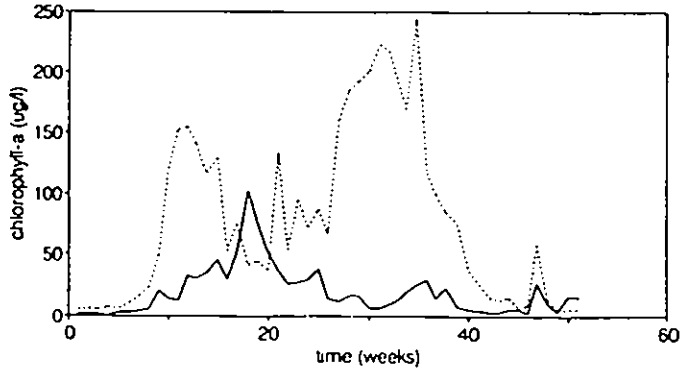
Validation plots 1976



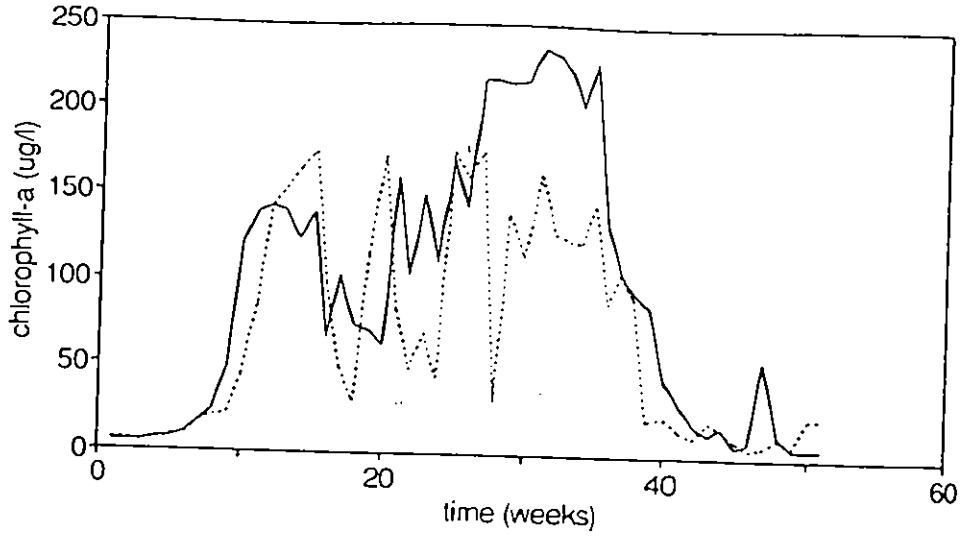
Validation reach 1



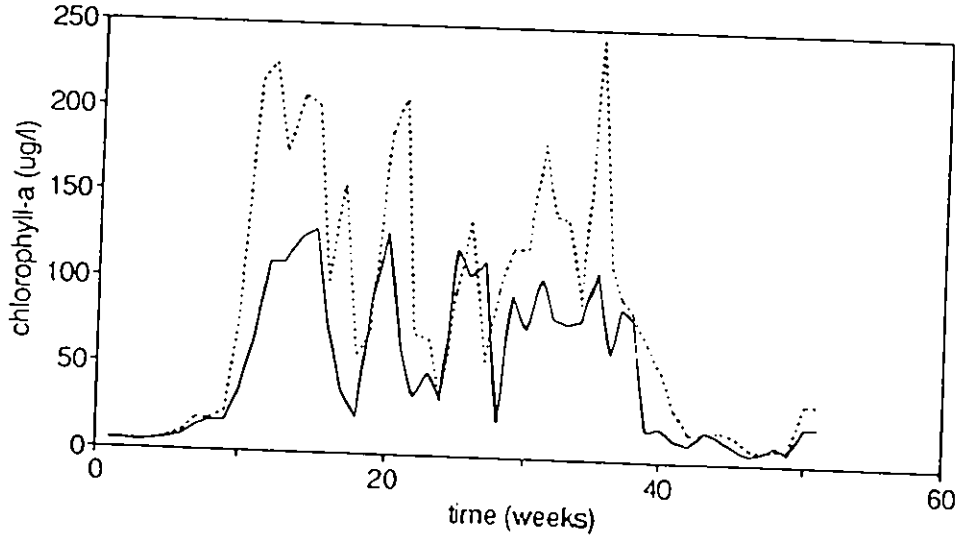
Validation reach 2



Validation reach 3



Validation reach 4



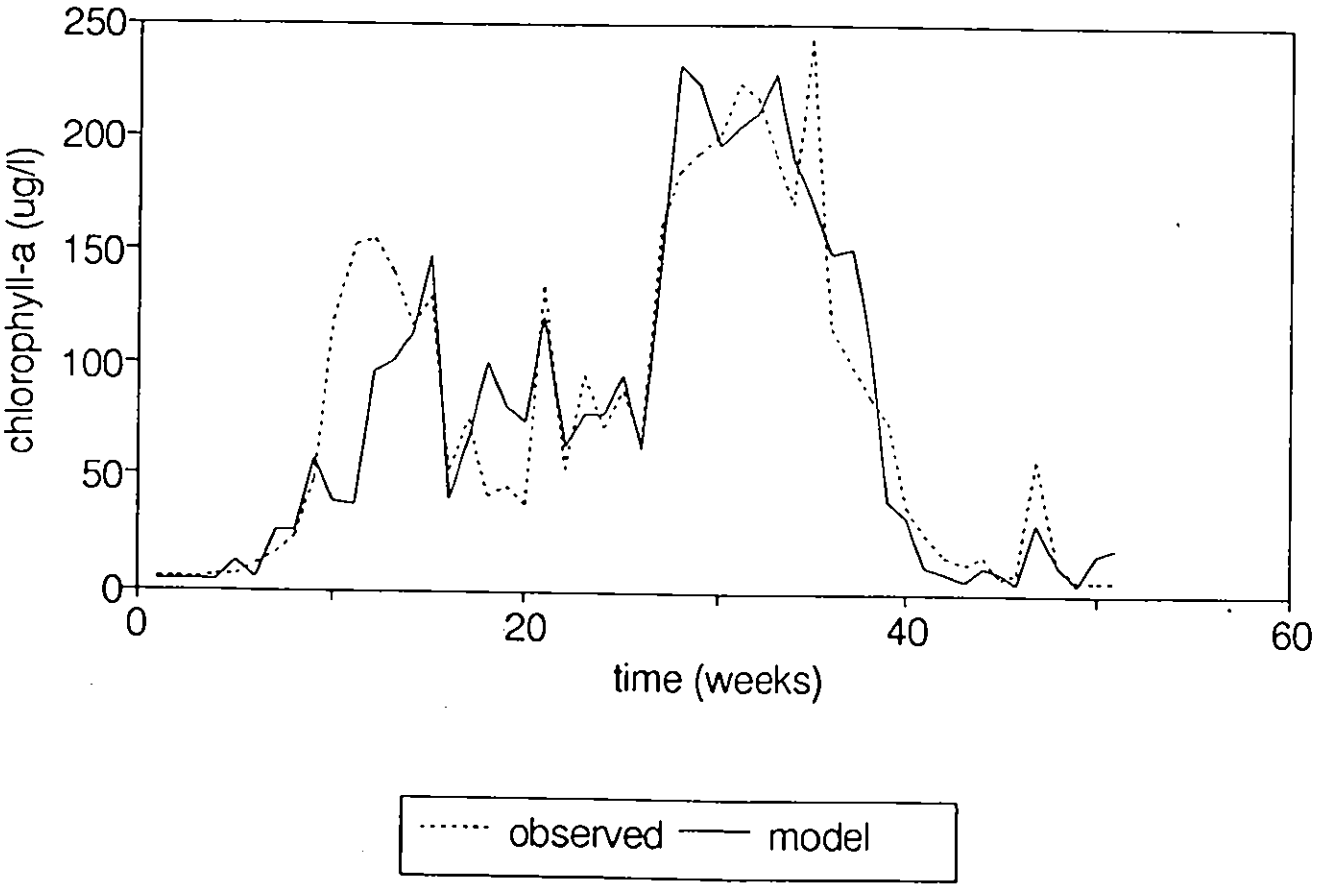
Validation reach 5

Calibration plot reach 3, 1976

Spring + autumn: $k_1 = 5$, $k_{2*} = 1.5$, $I_{opt} = 5000$, $\varepsilon_w = 0.8$

Summer: $k_1 = 1.3$, $k_{2*} = 0.8$, $I_{opt} = 5000$, $\varepsilon_w = 0.8$

$R_t^2 = 0.802$



Appendix F

Modified Differential Equations in Quasar

Dissolved Oxygen:

```
XP(4)=(U(4)-XO(4)+WEIR2)/TC
      +0.0899*K16*(1.04**(XO(7)-20.))*RI*XO(8)      Photosynthesis
      -(0.14+0.013*XO(8))*(1.04**(XO(7)-20.))       Respiration
       -K4*K6*XO(4)                                 Sediment respiration
       +K2*(CS-XO(4))                               Reaeration
       -K15*4.57*XO(6)                              Ammonia O2 demand
       -K1*XO(5)                                    O2 loss from BOD
```

Biochemical Oxygen Demand:

```
XP(5)=(U(5)-XO(5))/TC
       -K1*XO(5)                                    BOD deacy
       +0.0899*K10*XO(8)                            BOD contribution by algae
       -K18*XO(5)                                   loss of BOD by sedimentation
```

Algae:

```
EPS=0.80+0.016*XO(8)
RI=(2.718/(DEPTH*EPS))*(EXP((-SRAD/K19)*EXP(-DEPTH*EPS))-
*   EXP(-SRAD/K19))

IF(XO(7).LT.8.0)THEN
K16=0.0

XP(8)=(U(8)-XO(8))/TC
      +K16*(1.04**(XO(7)-20.0))*RI*XO(8)            growth
      -(K10+0.05)*XO(8)                             death and grazing
      -(0.10/DEPTH)*XO(7)                           sedimentation
```

When nutrients are limiting:
P<0.245 mg/l
K16=K16*(P/(P+0.005))
P=dissolved phosphorus (mg P/l)
N<1.225 mg/l
K16=K16*(N/(N+0.025))
N=ammonia nitrogen + nitrate nitrogen (mg N/l) (XO(2)+XO(6))
when both are limiting, the minimum factor

<u>Algae in the nitrogen cycle:</u>
(Values between parentheses are advised default values)
Contribution of algae to nitrogen, depends on the fraction of algal biomass that is nitrogen, algal death rate and algal biomass concentration (µg-Chl/l):
$dN/dt = +K10*\alpha*XO(8)$
α = nitrogen to algal ratio (mg-N/µg-Chl = 0.00833)
K10 = algal death rate

XO(8) = algal concentration (µg-Chl/l)

Uptake of nitrogen by algal growth.
Ammonia nitrogen (XO(6)):
$dN_1/dt = -F*\alpha*G*XO(8)$
G is effective algal growth, K16*F(N)*F(L)*F(T)
F is the ammonia preference factor: $P_nN_1/(P_nN_1 + (1-P_n)N_2)$
P_n = preference factor for ammonia nitrogen (0 to 1.0)
N_1 = concentration of ammonia nitrogen
N_2 = concentration of nitrate nitrogen
The ammonia preference factor is equivalent to the fraction of algal nitrogen uptake from the ammonia pool when the concentrations of ammonia and nitrate nitrogen are equal.

Nitrate nitrogen (XO(2)):
$dN_2/dt = -(1-F)*\alpha*G*XO(8)$
(Brown and Barnwell, 1987)

Algae in the phosphorus cycle:
(Values between parentheses are advised default values)
When algae die, algal P is released as organic P and inorganic P. Due to aerobic mineralisation in the water column organic P is converted to inorganic P. Organic P is present in a dissolved and a particulate form.
Uptake of P by algae occurs in the inorganic form only.

Organic P:
$dOP/dt = +f_{porg}*\beta*K10*XO(8)$
β = phosphorus to algal ratio (mg-P/µg-Chl = 0.000833)
f_{porg} = fraction algal P released as organic P (0.50)

Inorganic P:
$dIP/dt = -f_{porg}*\beta*G*XO(8) +(1-f_{porg})*\beta*K10*XO(8)$
(Aalderink, 1991)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