A note on the modelling of the algal blooms in the Vaal River: The silicon effect

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Abstract

In a recent article published in this journal, the authors described the basis of a mathematical model aimed to simulate the total planktonic biomass in a river. Taking only two fundamental environmental variables, light and temperature, into account, they developed a simple model that is able to give a good qualitative description of the winter algal bloom in the Vaal River (South Africa). However, some discrepancies between the simulated amplitude of certain algal blooms and field measurements were observed. In the present study, it is shown that this problem may, to a large extent, be solved by updating the model in order to take the Si uptake by diatoms into account.

Introduction

The prediction of the development of algal blooms in a river is of great importance in water resource management (Walmsley and Butty, 1983; Pieterse, 1986). Recently Cloot et al. (1992) introduced a mathematical model for algal growth with the intention that it should eventually be able to assist researchers and the relevant authorities by providing a tool which can lead to a better understanding of aspects of algal growth, and which might enable meaningful short- and long-term water quality predictions. In its original version, algal growth was modelled by taking only water temperature and underwater light climate variations into account. Within this framework, and assuming that assemblages containing up to N algal groups are responsible for the blooms, we derived a basic scheme that may be used for the modelling of algal growth. This scheme is illustrated in Fig. 1.

The transcription of the scheme in Fig. 1 in terms of mathematical relations leads to a system of N pairs of coupled non-linear differential equations:

$$\begin{aligned} \dot{x}_{1i} &= [-k_{Di} + k_{Si}) + k_{Gi}(T, I, \underline{K}_j; j = 1, N)]x_{1i} \\ \dot{x}_{2i} &= k_{Di}x_{1i} - k_{Si}x_{2i} \end{aligned} \qquad (1)$$

that depend explicitly on parameters which could be classified in two categories, namely environmental variables and variables that are specific for a particular algal group. The environmental parameters that were needed for this basic model, are given in Table 1.

Furthermore, the reactions of algae to variations in environmental variables differ from group to group (Hoogenhout and Amesz, 1965), and the sensitivity of the i-th algal group can be represented by a set of parameters $\underline{K}_i$ of which the components are given in Table 2.

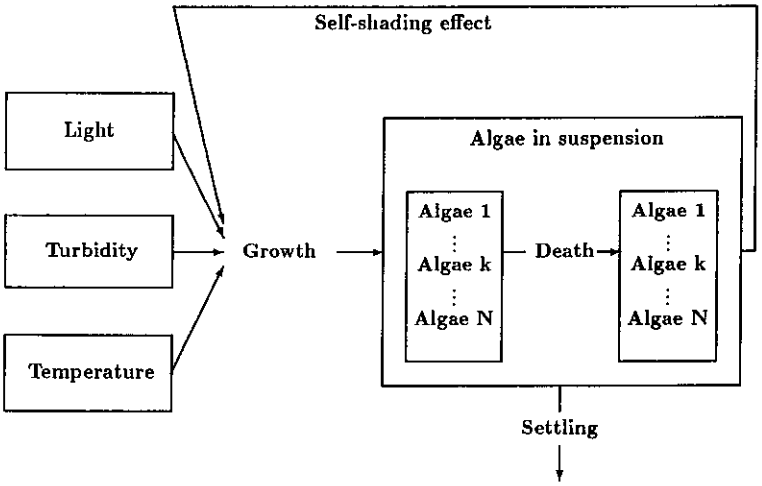

Figure 1
A schematic representation of the basic light-temperature Vaal River N-algal growth model

TABLE 1
ENVIROMENTAL PARAMETERS

I_{max}	:	maximal irradiance available on the water surface
$\mu(t)$	:	cosine of solar zenith angle
T	:	the water temperature
$S(t)$	:	total concentration of inorganic material suspended in the water
z_0	:	depth of the mixed layer
k_w	:	light extinction coefficient for pure water
c_s	:	light extinction coefficient for suspended inorganic solids

This model was calibrated on data available from the Vaal River and tested on *in situ* measurements from the Stilfontein site, during a three year period starting January 1985.

During the winter to spring period of each of these years, two

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TABLE 2
PARAMETER SET REPRESENTING THE I-th ALGAL CATEGORY (THE INDEX "I" HAS BEEN OMITTED HERE FOR CONVENIENCE)

I_{opt}	optimal light intensity for growth
k_G	maximum algal growth rate
T_{opt}	optimal temperature for algal growth
T_{min}	minimum temperature for algal growth
k_D	algal dying rate
k_S	algal settling rate
k_x	self-shading coefficient for algae

algal blooms were observed. The first of these blooms was due mainly to diatoms, while the second was mainly caused by green algae. Assuming that only assemblages containing two algal types were possible, and using the weekly averaged water temperature and suspended inorganic solid concentration as data, the system of Eq. (1) was solved numerically for the winter-spring period of each of the three years and the total algal biomass was computed in terms of the chlorophyll-a concentration. As an example, Figs. 2a-c show the model simulation (solid line) together with measurements *made at Stilfontein during 1985,1986 and 1987, respectively.*

The agreement between simulated and measured values was, overall, fairly good. However, during the winter algal bloom period of 1985 and 1986 better results were obtained in the modelling of the second algal bloom than the first one. In the following sections we will show how this situation can be improved if an additional step is included in the modelling process by explicitly including the possible effects of variations in dissolved Si concentration in the water on the growth coefficient of diatoms.

Diatoms, silicon uptake and dissolved silicon concentration

Unlike other types of algae diatoms are able to absorb the element Si dissolved in the water in the form of orthosilisic acid $Si(OH)_4$ (Werner, 1977). The availability of this element has been proved to be essential in the formation of the frustules of diatom cells, which act as a shield against predators and parasites present in the environment, and also for protection against disturbances of a mechanical nature (Eppley, 1977). Should the dissolved Si concentration in the water be depleted, diatom growth and development are negatively affected.

Since only algae belonging to the diatom group are able to affect the concentration of dissolved Si in the water, the monitoring of this component of the ecological system during an algal bloom could also provide an elegant and powerful means to retrieve, a *posteriori, the extent to which algae belonging to the diatom group* were responsible for an algal bloom. It should be noted that the viability of Si as an indicator of the presence of diatoms is higher than any other nutrient. In particular, it is far more effective than simply taking into account the water temperatures observed during the bloom, because there is an overlap between the range of temperatures favourable for growth of diatoms and green algae. Furthermore, if it is assumed that the necessary information on the saturation concentration of dissolved Si in the water is available, the measurement of available Si concentrations in the water will allow the researcher to obtain information about the relative abundance of diatoms during a mixed bloom, i.e. an algal bloom realised by a combination of algae belonging to more than one algal group.

The influence of the dissolved Si concentration in the water on the growth of diatoms is implemented in the model represented in Fig. 1 in two phases: In the first phase, the mechanical and chemical processes determining the dissolved Si concentration in the water are considered. This concentration will be referred to as the

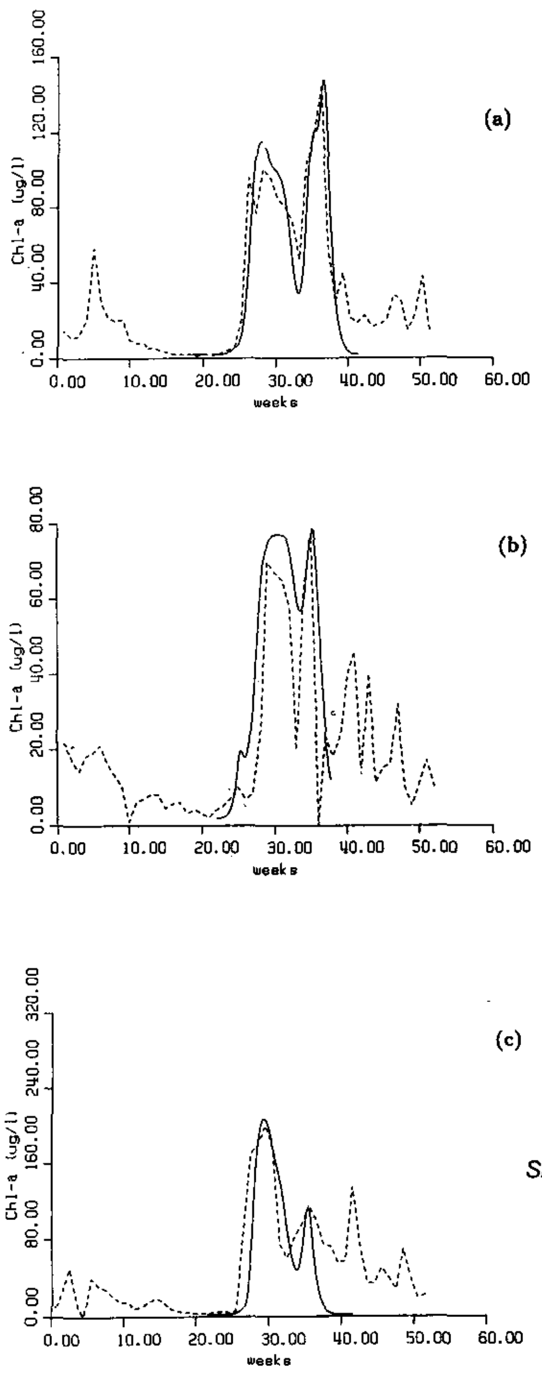

Figure 2
Simulated (solid line) and actual (dashed line) total chlorophyll-a concentration in the Vaal River at Stilfontein during the winter-early spring period of
(a): 1985
(b): 1986
(c): 1987
(Week 0 starts on 1 January)

TABLE 3
BALKFONTEIN: MEASURED DATA FOR 1986-1987

Date	chl-a (µg/ℓ)	Algal group	Temp. (°C)	Si (µg/ℓ)	Q (m^3/s)	TUR (NTU)
86-02-18	25	Green+Diatoms	26	2.8	17	7.4
86-04-03	22	Green+Diatoms	21	3.83	12	12.2
86-06-24	10*	?	14	3.37	15	?
86-08-29	65	Diatoms	14.5	0.52	25	28
86-10-20	40	?	1.8	1.87	22	12
86-12-09	35	Green+Diatoms	24	4.4	17	?
87-02-26	38	Green+Diatoms	27	2.57	1.6	21
87-03-24	25	?	24	2.56	1.5	23
21-04-21	25*	?	23	4.94	4	11
87-05-25	30*	Green	20	4.07	0.7	12
87-06-30	20*	?	10	3.14	20	4
87-08-04	80	Diatoms	11.1	0.62	26	16
87-08-17	110	Diatoms	15	0.56	27	11
87-09-16	61	Diatoms+Green	21.5	0.51	12	14
87-10-13	83*	Green	20	4.14	13	52
87-11-18	86*	Green	24	4.71	32	41
87-12-08	83*	Green	26	4.98	136	57

saturation-concentration, Si^{sat}. The second phase consists of the modelling of the Si uptake by diatoms, with particular emphasis on the influence of Si uptake by diatoms on the dissolved Si concentration in the water, and the effect of dissolved Si concentration on the diatoms' growth coefficient.

Dissolved silicon content of the water as a product of a mechanical and chemical process

It is well accepted that the Si is taken up by diatoms in the form of orthosilisic acid, i.e. $Si(OH)_4$ (Werner, 1977). Thus, the following path for Si uptake by diatoms is considered possible:

$$SiO_2 + 2H_2O \Leftrightarrow Si(OH)_4 \rightarrow \text{Diatom uptake}$$

Assuming at first that the concentration of dissolved SiO_2 in the water body is governed by a chemical process only, the following chemical equilibrium can be considered:

$$SiO_2|_{amorphous} + 2H_2O \Leftrightarrow Si(OH)_4 \tag{2}$$

This chemical reaction is characterised by the equilibrium constant:

$$K(T)|_{am} = \frac{[Si(OH)_4]}{[SiO_2][H_2O]} \tag{3}$$

which, assuming that the infinite dilution hypothesis is applicable, may be reduced to:

$$K(T) \approx [Si(OH)_4] \tag{4}$$

According to the literature (Stumm and Morgan, 1970), the value of K can be considered insensitive to pH variations (up to pH≈9), and is pressure-independent (as long as the pressure is less than 1 000 atmospheres) but, like most chemical equilibrium constants, it is a function of the (absolute) temperature.

The temperature dependence of this equilibrium coefficient $K(T)$ is therefore modelled, in agreement with classical chemical practice, by means of the Arrhenius equation:

$$K(T) = Ae^{-\frac{\Delta H_f}{RT}} \tag{5}$$

where ΔH_f is the enthalpy of formation of $Si(OH)_4$, R is the universal gas constant, T is the absolute temperature (expressed in degrees Kelvin), while A is a constant.

For a given substance, the enthalpy of formation has a fixed value and Eq. (5) contains only one unknown parameter, namely A. If only chemical processes are taken into account, this remaining parameter will be a constant. However, rivers are dynamic systems and it may be possible that the movement of the water and its turbidity as well as the chemistry involving other elements dissolved in the water body perturbs the characteristics of the chemical equilibrium as described by the Eq. (4). Therefore, in an attempt to account for the possible influence of these factors, we assume *a priori* that parameter A is no longer a constant, but could be an (unknown) function of the discharge Q and/or the turbidity (TUR) of the water, i.e.:

$$A = A(Q, TUR)$$

to be determined. In order to gain some information on this function, in the context of the Vaal River, the environmental data available from the Balkfontein site for the period 1986 to 1987 were taken in account, namely: water temperature, Si concentration, flow, turbidity and chlorophyll-*a* concentration (see Table 3).

At this stage of the modelling process, only the data corresponding to either a low concentration of algae (in the Vaal River context) or to an algal bloom realised by algae not belonging to the diatom group are relevant (these data are indicated by an asterisk in Table 3). The collection of relevant data sets is given in Table 4.

With the help of Eqs. (4) and (5) it is possible to eliminate the

TABLE 4
SI SATURATION CONCENTRATION : FIELD DATA

Temperature (°C)	Si^{exp} (10^{-3} M/ℓ)	Q (m³/s)	TUR (NTU)
14	0.1204	15	
23	0.17643	4	11
20	0.14536	0.7	12
10	0.112143	20	4
20	0.14786	13	52
24	0.168214	32	41
26	0.17786	136	57

effect of temperature from the field data to get an idea of the value of *A(Q,TUR)* by means of the following equation:

$$\frac{Si^{exp}}{e^{\frac{-\Delta H}{RT_{exp}}}} = \frac{K(T_{exp})}{e^{\frac{-\Delta H}{RT_{exp}}}} = A(Q)|_{exp} \qquad (6)$$

The results of this computation are given in Table 5.

TABLE 5
EXPERIMENTAL VALUES OF A(Q, TUR)

Si^{exp} (10^{-3} M/ℓ)	A (M/ℓ)	Q (m³/s)	TUR (NTU)	Si^{proj} (10^{-3} M/ℓ)
0.1204	1.856	15		0.1234
0.17643	2.029	4	11	0.1654
0.14536	1.839	0.7	12	0.1503
0.112143	1.982	20	4	0.1076
0.14786	1.871	13	52	0.1503
0.168214	1.875	32	41	0.1707
0.17786	1.862	136	57	0.1816

From this reduced set of data, it is clear that neither the magnitude of the flow nor the turbidity have a significant influence on parameter *A*, at least for the period covering the years 1986 to 1987 and at the Balkfontein site. The value of the coefficient, *A*, is thus chosen as the average of the values presented in Table 5 i.e.:

$$A(Q) = A = 1.902\ M/\ell \qquad (7)$$

The projected dissolved Si values, obtained by means of Eq. (6), are given in the last column of Table 5. Comparing these with the measured values (see Column 1, Table 5), it is clear that a good agreement between observed and predicted values is achieved whenever the concentration in algae belonging to the diatom group is not too high. However, should the concentration of diatoms increase, the effect of these algae on the dissolved Si concentration has to be taken into account.

Modelling the Si uptake by diatoms

During the last two decades, mechanisms involved in the uptake of Si by diatoms have been studied. Some general features of primary importance when modelling his aspect of algal metabolism, are the following. The rate of Si uptake by a diatom cell depends on the species involved as well as on the orthosilicic acid concentration observed in the immediate vicinity of the cell. Usually, the rate of uptake is a non-linear increasing function of the Si concentration which exhibits a saturation phenomenon beyond a relevant level of dissolved Si, Si^{cr}_{up} and which is discontinued if the orthosilisic acid concentration in the water falls below a certain level, Si^{min}_{up} (Jorgensen,1979). This behaviour suggests that a relevant function *to model Si uptake by a given diatom cell, "i", may be of the form:*

$$Vi = \begin{cases} V_{max\,i} & if \quad Si \geq Si^{cr}_{up_i} \\ V_{max_i} L(Si, Si^{cr}_{up_i}, Si^{min}_{up_i}) & if \quad Si^{cr}_{up_i} > Si \geq Si^{min}_{up_i} \\ 0 & if \quad Si \geq Si^{min}_{up_i} \end{cases} \qquad (8)$$

where $V_{max\,i}$ represents the maximum rate for Si uptake, which is only reached if the dissolved Si concentration exceeds the critical level Si^{cr}_{upi}. The transfer function L modulates this maximum rate of uptake when the dissolved Si concentration is below the optimal level. The behaviour of this function is illustrated in Fig. 3, for a realistic choice of the parameters (Werner, 1977):

$$\frac{Si^{exp}}{e^{\frac{-\Delta H}{RT_{exp}}}} = \frac{K(T_{exp})}{e^{\frac{-\Delta H}{RT_{exp}}}} \approx A(Q)|_{exp}$$

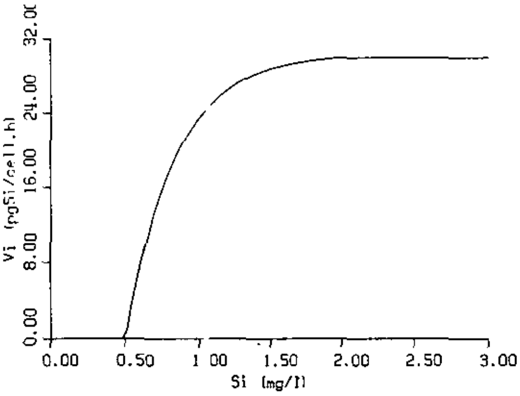

Figure 3
Evolution of the uptake function V_i with Si^{sat} = 2 mg/ℓ, V_{max} = 30 pg Si/cell·h

As far as the order of magnitude of the different parameters arising in the function, *L*, is concerned, little information is available in the literature. Therefore, only an overall estimate for the range of variation of the rate of uptake:

$$V_{max_i} \in [10^{-1} - 10^{-5}]\, mg\, Si(\mu\, gchl - a.h)^{-1}$$

could be reached. On the other hand, the field data seem to indicate that the following orders of magnitude for the remaining parameters, are acceptable:

$$Si^{cr} \approx 2mg\, Si\, /\, l$$
$$Si^{min} \approx 0.5mg\, Si\, /\, l. \qquad (9)$$

Note that these values are derived from a rather small set of experimental data and that more information on this aspect of the problem is necessary. In particular, the suggested order of magnitude for the minimum concentration value for possible Si uptake by diatoms, 0.5 mg $Si{\cdot}\ell^{-1}$, is rather high and should probably be seen as an upper bound for the parameter.

Combining the two aspects of the problem, i.e. the uptake of Si by diatoms and the existence of a dissolved Si saturation concentration, Si^{sat}, we obtain a differential equation describing the behaviour of dissolved Si in the water:

$$\frac{dSi}{dt} = \mathrm{Prod}_{Si}(Si^{sat}(T), Si, k_{Si}^{prod}) - \sum_{i=diatom} V_i x_{1i}, \qquad (10)$$

where Si^{sat}, the saturation concentration (in the absence of diatoms), is defined by Eq. (5), while the V_i's are given by (8). Finally, the coefficient, k_{Si}^{prod} is the inverse of the characteristic time of restitution for saturated Si concentration under the condition that no diatoms are present in the water. From field measurements, it appears that a relevant order of magnitude for this coefficient, in the Vaal River context, is:

$$k_{Si}^{prod} \approx 0.1429\ day^{-1} \qquad (11)$$

This means that the time of recovery for the Si concentration is at least about one week. Note that, once again, this additional equation describing the evolution of dissolved Si concentration in the river is completely non-linear and coupled to other variables like the temperature and the concentration of living diatoms.

Up to now, only the effect of diatoms on the dissolved Si concentration has been considered. The effect of dissolved orthosilicic acid levels in the water on the behaviour (the growth) of different diatom species must also be considered. Indeed, if the algae have to grow in an environment where the Si concentration is unfavourable, the metabolism of these algae will be affected and their growth rate will deviate from its optimal value. Because metabolic activities and cell divisions rate are correlated, it is natural to consider that, for a given diatom i, the growth rate will be affected in a way similar to the Si uptake rate, when the concentration of the orthosilisic acid is varied. This suggests that the effect of Si concentration on the growth rate coefficient can be taken to be of the form:

$$k_{G_i}(I,T,Si) = \begin{cases} k_{G_i}(I,T)L(Si, Si_{G_i}^{cr}, Si_{G_i}^{min}) & if \quad Si_{G_i}^{cr} \geq Si > Si_{G_i}^{min} \\ k_{G_i}(I,T) & if \quad Si \geq Si_{G_i}^{cr} \\ 0 & if \quad Si \leq Si_{G_i}^{min}. \end{cases} \qquad (12)$$

This function identifies completely with relation (8). However, the coefficient values are allowed to differ from those relevant to the Si uptake, i.e. it is possible that Si_{upi}^{cr} , Si_{upi}^{min} may differ, usually slightly, from Si_{Gi}^{cr} , Si_{Gi}^{min} . The distinction between coefficients is made necessary in order to account for the fact that most of the diatom species are capable of absorbing Si in excess and then using the reserve to prevent or delay the effect of Si depletion, should it occur (Werner, 1977). Furthermore, the coefficient k_{Gi}, (I, T)identifies with the growth rate coefficient depending only on light and temperature, as defined in earlier studies (Cloot et al., 1992).

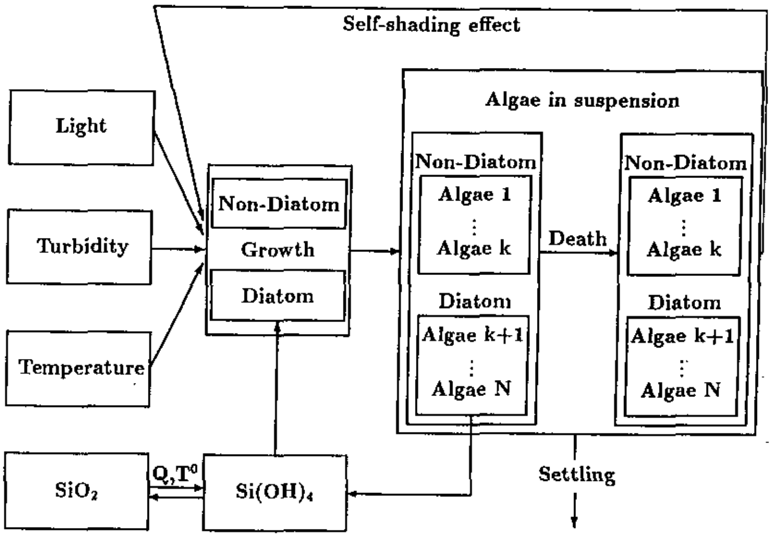

Figure 4

Vaal River N-algal growth model including the dissolved Si effect: A schematic representation

The mathematical model: Updated version

When Si uptake by diatoms is taken into account, the schematic representation of the basic version of the mathematical model presented in Fig. 1 is no longer valid and has to be replaced by the scheme illustrated in Fig. 4.

The updated version presented in the schematic representation has to be implemented in a basic set of equations, (1), which now takes the form of a system of $\underline{2N+1}$ non-linear differential equations:

$$\dot{x}_{1i} = [-k_{Di} + k_{Gi}(T, I, Si, \underline{K}_j; j=1,n)]x_{1i}$$
$$\dot{x}_{2i} = k_{Di}x_{1i} - k_{Si}x_{2i}$$
$$\dot{Si} = \mathrm{Prod}_{Si}(Si^{sat}(T), Si, k_{Si}^{prod}) - \sum_{i=diatom} V_i x_{1i}$$

Numerical simulation

In order to illustrate the influence of Si depletion in the river on diatom growth, the same computational experiments which were performed with the help of the basic light-temperature dependent model described in an earlier section but including the possible effect of Si concentration on the rate of algal growth, are performed. As mentioned in the introduction, it is known that the winter algal blooms, in the Vaal River context, are usually initiated by diatoms, followed by green algae. In the light of this experimental evidence, we thus assume that this pattern holds in our particular cases and consider that the first alga appearing during the winter periods 1985 to 1987 is a diatom, i.e. sensitive to Si variations in the water, while the second algal bloom is due to a non-diatom alga. Keeping the light and temperature parameters of the first alga at their original values, we define an additional subset of parameters relating to Si uptake (see Table 6) and the program is rerun to see if Si effects could account for discrepancies observed within the framework of the original light-temperature model.

The results of these numerical experiments are illustrated in Figs. 5a-b for the winter periods of 1985 and 1986, respectively. Comparing these results with the results obtained from the basic

TABLE 6
OPTIMAL PARAMETER SET FOR THE LIGHT-TEMPERATURE AND LIGHT-TEMPERATURE-SI DEPENDENT MODELS

	Light-temperature model				Light-temperature-Si model			
	1985		1986		1985		1986	
Parameter	**Alga 1**	**Alga 2**	**Alga 1**	**Alga 2**	**diatom**	**non-diat.**	**diatom**	**non-diat.**
k_G	1.43	1.65	1.28	1.46	1.43	1.68	1.28	1.40
k_D	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
I_{opt}	0.12	0.075	0.12	0.08	0.12	0.075	0.12	0.08
T_{opt}	11	15	10	13	11	15	10	13
T_{min}	0	5	0	5	0	5	0	5
Si_{up}^{cr}					2		2	
Si_{up}^{min}					0.5		0.5	
V_{max}					0.007		0.01	
Si_G^{cr}					1		1	
Si_G^{min}					0.5		0.5	

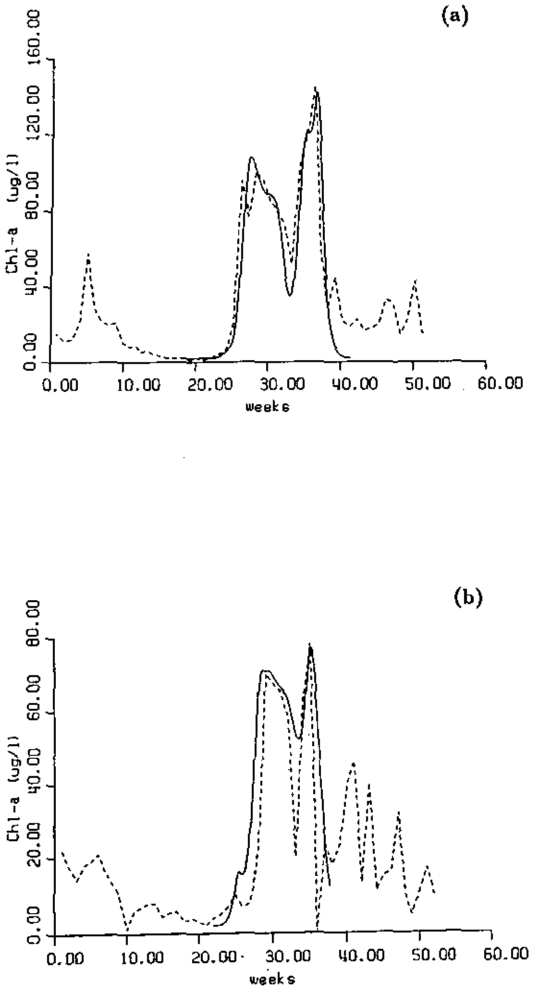

Figure 5
The same as Fig. 2a-b, except that Si uptake by the diatoms is taken into account

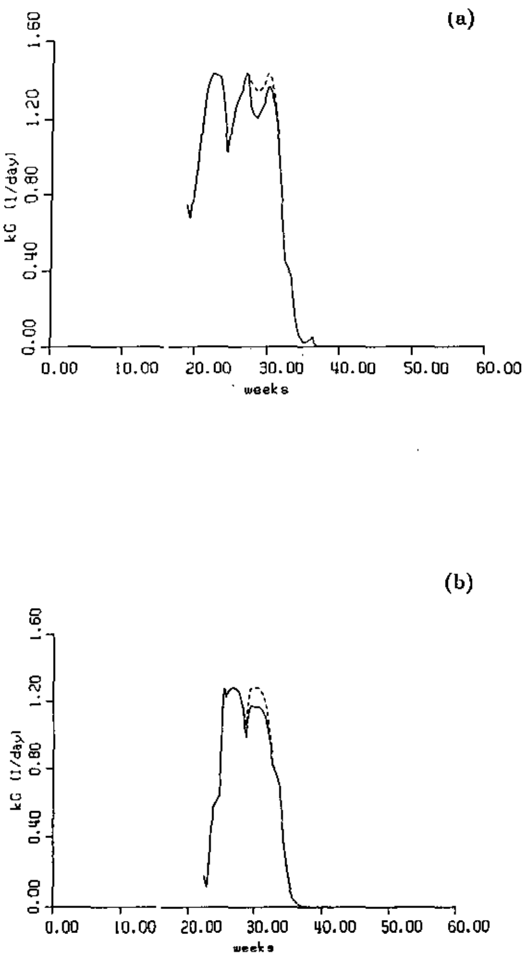

Figure 6
Time-evolution of the growth coefficient of the diatoms for the years (a): 1985; (b): 1986, assuming that : only light and temperature affect this coefficient (dashed line); light, temperature and Si determine the amplitude of k_G (solid line). Note that most of the time solid (Si) and dashed lines (no Si) overlap and then only a solid line is visible.

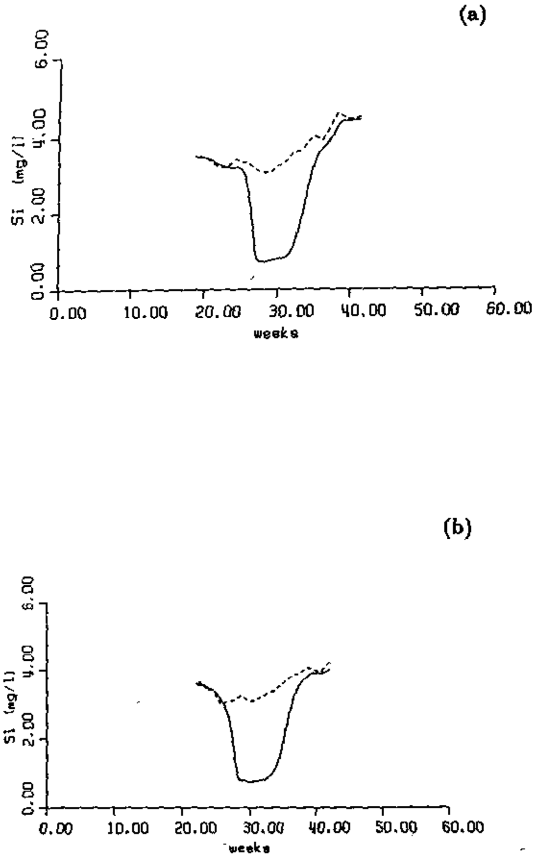

Figure 7

Evolution of dissolved Si concentration during the winter algal blooms as predicted by the model: (a): 1985; (b): 1986. The dashed line represents the saturation concentration reachable in absence of diatom growth while, the solid line represents dissolved Si curve as computed by the model.

model (see Fig. 2a-b), it is clear that the taking into account of the effects of Si markedly improves the fitting of the calculated values to the measured values.

If the evolution of the values of the growth coefficient of algae 1 (i.e. the diatoms) for both cases (see Fig. 6a-b), together with the projected behaviour of the dissolved Si concentration in the water is computed (see Fig. 7a-b), it is observed that, as long as the diatom concentration stays at a low level, depletion of Si by algal uptake is more or less counterbalanced by Si production, while the Si concentration remains above the saturation concentration. Also, no effect on the growth coefficient is observed. However, with increasing diatom concentrations, the balance can not be maintained and Si depletion occurs to such an extent that it becomes a limiting factor for growth. In this case the dissolved Si concentration becomes a limiting factor for growth.

Conclusions

By taking into account the possible effects of variations in dissolved Si concentration in the water, it was possible to improve the quality of the simulation of algal growth and algal blooms in the Vaal River. However, some discrepancies still remain between simulated and measured values of the total chlorophyll-*a* concentrations, that are not explained by the Si effect alone. Thus it is obvious that the influence of other factors will have to be implemented in the mathematical model. The next steps in the development of the model would be to include the effect of salinity, pH, phosphate and nitrate concentration, as well as that of dissolved carbon dioxide. The planned approach should give a better quantitative agreement between simulated and observed values, and would also give a better indication of the overall interaction between the algae and their environment.

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