SIMPLIFYING DYNAMIC RIVER WATER QUALITY MODELLING: A CASE STUDY OF INORGANIC NITROGEN DYNAMICS IN THE CROCODILE RIVER (SOUTH AFRICA)

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ABSTRACT

Increasing water scarcity in many countries provides a strong impetus for investments in water quality remediation at the basin or sub-basin scale as a means to increase water availability. The application of mathematical river water quality modelling, as a support tool to evaluate remediation options, is often limited by the availability of reliable data. Current proposals to use the River Water Quality Model number 1 (RWQM1) are hampered by its relative complexity and large data requirements, with the result that use of such model is often not economically feasible, especially in developing countries. However, by simplifying this model to suit specific applications, the general water quality situation of a river can still be predicted with limited data. The ultimate goal of this study is to develop a simple dynamic river water quality model that is compatible with activated sludge models and which can be used for integrated water quality modelling studies in the future. During the present study, a simplified river water quality model was derived from the available RWQM1 model and used to investigate the daily dynamics of nitrate and ammonia nitrogen concentrations in the Crocodile River in South Africa. Using a modelling concept based on continuously stirred tanks in series, the simulation results for two years agree well with the measured seasonal dynamics of nitrate and ammonia concentrations in the river system. The model is most sensitive to the concentration of nitrifiers and to hydraulic parameters.

KEYWORDS

Crocodile River, dynamic, river, RWQM1, sensitivity analysis, water quality modelling

INTRODUCTION

The challenge of using mathematical modelling, as a support tool to evaluate water quality remediation options, in developing countries is well documented (Ongley and Booty, 1999). However, modelling is expensive, requires substantial investments in reliable data, development of scientific capacity and a relatively sophisticated management culture that are often not found in developing countries. Nevertheless, new developments in water quality management polices and strategies require prediction of the fate of in-stream pollutants, as well as estimates of the likely effects that the resultant water quality may have on recognized water uses. The complex relationships between waste load inputs, and the resulting water quality responses in receiving water bodies are best described with mathematical models.

River water quality models are used extensively in research as well as in the design and assessment of water quality management measures and several types of water quality models are available. The complexity and number of state variables of these models increase from the simplest Streeter-Phelps (Oxygen sag curve) to extended models such as QUAL1, QUAL2, ISIS, DUFLOW and MIKE11. Importantly, none of these models use bacteria as state variables despite the fact that bacteria determine and control the rates of biotransformation processes. As a result, these models usually need to be modified for application in water quality studies. Moreover, an integrated water quality modelling approach requires a river water quality model that can be connected directly to, and is compatible with, typical Activated Sludge wastewater treatment plant Models (Reichert et al., 2001).

Accordingly, the IWA Task Group on River Water Quality Modelling have proposed that the River Water Quality Model number 1, RWQM1 should be adopted for general use (Reichert et al., 2001). This model is compatible with the existing IWA Activated Sludge Models (ASM-1, ASM-2 and ASM-3, Henze et al., 1987, Henze et al., 1995, and Gujer et al., 1999 respectively), and contains bacterial biomass as state variables. However, RWQM1 is considered to be too comprehensive and complex to apply directly in many situations, for example in developing countries where there are limited available data. Often, one is then limited to a simple river water quality model that still describes components of the C, O, N and P cycles and is still compatible with ASM1.

The ultimate goal of this study is to derive a simple dynamic river water quality model that is compatible with activated sludge models (ASM), so that it can be used for integrated river water quality modelling studies. Accordingly, a simplified river water quality model was derived from the available RWQM1 model, and was used to investigate the dynamics of nitrogen concentrations in downstream reaches of the Crocodile River in South Africa.

STUDY SITE

The Crocodile River catchment is located in the Mpumalanga Province of South Africa (Figure 1), where it comprises 1.2% of the total area of the country and supports one of South Africa's largest and most important irrigation areas. The total irrigated area of approximately 132,000 ha comprises some 91,000 ha of vegetables and other crops, 21,000 ha of sugarcane and 20,000 ha of citrus orchards (DWA, 1995, Van der Zel, 1977). The total population residing in the catchment has been estimated to be 550,600 in the year 2000 and 632,500 in the year 2005 (Ashton et al., 1995), with approximately 76% of these residents located in urban areas. The Crocodile River catchment is well known for its scenic attractions, high tourist potential, and sensitivity to environmental degradation.

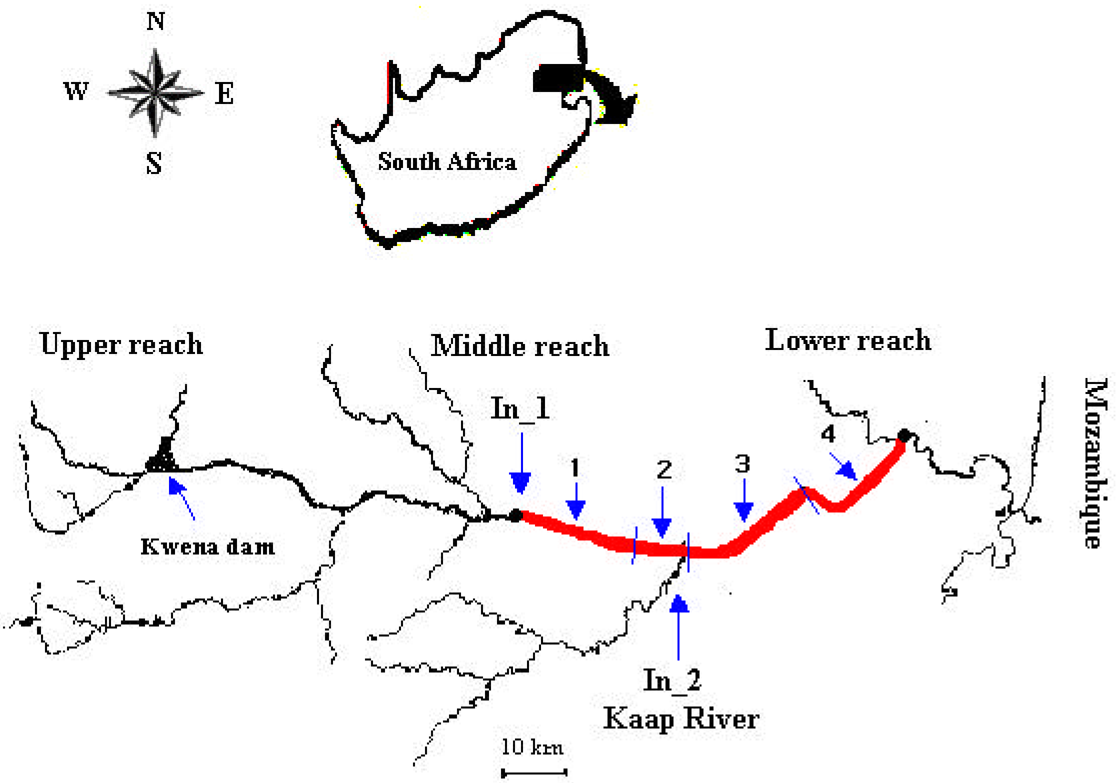

Figure 1. Map of the Crocodile River system: The thick solid line indicates the sensitive river section included in the model. In_1 and In_2 are model inputs; 1- 4 are river compartments. Only selected major tributaries are indicated in this figure.

By South African standards, the Crocodile River is considered to be a relatively large river. The river has a total length of some 320 km and drains a catchment area of about 10,440 km^2, before joining the Komati River and flowing into Mozambique. Annual rainfall varies from 1200 mm in the mountainous area at the head of the catchment to 600 mm in the eastern Lowveld. The mean annual precipitation is 880 mm, with 80% of all rainfall received as convective thunderstorms during the warm summer months of November and April.

River water quality is influenced by pollutants discharged from industrial and domestic wastewater treatment plants, as well as by runoff and return flows from the extensive areas of irrigated agriculture. The middle reaches of the catchment contain a total of 30 conventional sewage treatment works whose effluent is directly discharged to the middle reaches of the Crocodile River and its tributaries. As a result, downstream sections of the river often experience serious water quality problems, particularly, the presence of toxic heavy metals, increased salinity values and escalating eutrophication. Since the river is relatively large, and very few measured data are available regarding pollution loads in the upper catchment, a section of some 70 km of the downstream reaches of the Crocodile River was selected for this study. The chosen section represents the most sensitive portion of the river, where nitrate and ammonia concentrations often exceed the recommended maximum limits of 0.5 mg/l (nitrate) and 0.03 mg/l (ammonia) for oligotrophic systems (DWA, 1993; Ashton et al., 1995). Within the selected reach, the river forms meanders that are shallowly incised into a wide sandy riverbed (20 - 30 m). This slow flowing reach is prone to extensive infestations of water hyacinth, particularly in the slower-flowing portions near several flow-gauging weirs. These dense mats of water hyacinth occasionally cause fish kills by depleting the dissolved oxygen underneath the mats. This study focuses mainly on non-point sources of nitrogen pollution from mining and agricultural activities. For the river section under consideration, daily flows and monthly water quality data for NO_3-N+NO_2-N, NH_4-N and PO_4-N were available, and a data set covering a two-year period (1989-1990) was chosen for model evaluation.

MODEL FORMULATION

In the process of simplifying the model, the two fundamental parts of river water quality models, namely the hydrodynamic and conversion processes, are described separately. The complex hydrodynamic river model was simplified by using the well-known Continuously Stirred Tank in Series (CSTR) approach in which the river is described as a series of river compartments (tanks), each of which is assumed completely mixed (Reichert et al., 2001). The water balance equation in the simplified model for a single tank is:

$$\frac{dV}{dt} = Q_{in} - Q_e - ET * A$$

where V volume of the tank (L^3);
Q_{in} influent flow rate to the tank [L^3T^{-1}]
Q_e effluent flow rate from the tank [L^3T^{-1}]
ET evapotranspiration from the river stretch calculated by the Hargreaves method [LT^{-1}]
A surface area of the river tank [L^2]

The inclusion of an evapotranspiration factor (ET) in the model is very important, particularly when dealing with long and wide rivers like the Crocodile River where the annual mean evapotranspiration loss for the catchment (1800 – 2000 mm) exceeds mean annual precipitation (< 800 mm) by a wide margin (DWAF, 1995). Because evapotranspiration leads to an increase in the concentration of constituents in the river, the impact on the river water quality should not be neglected. Excessive salinity, for example, is one of the adverse consequences in downstream reaches of the catchment. Human activities such as irrigation and mining are the main sources of salinity in the Crocodile River. The measure of salinity (Electric Conductivity, EC) increases with river length (from about 13 mS/m at 14 km, to 40 mS/m at a distance of 270 km from Kwena Dam (data for July 1990).

Since it is relatively wide (more than 20 m), one can assume that the river cross-sections are approximately rectangular, and the effluent flow rate from each “tank” can be calculated using the power function approximation according to equation 2. The flow velocity is variable and perturbations are propagating downstream with this variable speed (equation 3).

$$Q_e(t) = a\,h^b(t)$$

$$v(t) = \frac{Q_e(t)}{A_{cross}(t)}$$

where *h (t)* the hydraulic depth at time *t* [L] = $V(t)/A_{cross}(t)$
ß parameters estimated from stage flow relations [-]
?(t) flow velocity at time *t* [LT^{-1}]
$A_{cross}(t)$ cross-sectional area at time *t* [L^2]
t the time variable [T]

The conceptual one-dimensional river water quality model in a variable volume river stretch is expressed as the mass balance:

$$\frac{d(VC)}{dt} = Q_{in}C_{in} - Q_eC + Vr$$

where C_{in} influent concentration [ML^{-3}]
C effluent concentration [ML^{-3}]
r reaction rate [$ML^{-3}\,T^{-1}$]

Based on equations 1 and 4 another interesting equation can be derived as

$$\frac{dC}{dt} = \frac{Q_{in}}{V}C_{in} - \frac{1}{V}(Q_{in} - ET * A)C + r$$

As illustrated in equation 5, the concentration dynamics in a tank with variable volume is not dependent on the effluent flow rate Q_e but rather depends on the influent flow rate Q_{in} and evapotranspiration *ET*. This means that the mass balance is calculated with the same equation as for a tank with constant volume, but now a time dependent volume is used. The model formulation requires the hydraulics calculations to be performed separately and prior to the calculation of the mass balance.

Regarding the conversion process, which describes changes in constituent concentrations due to biological, chemical, biochemical, and physical processes, many models are available for use in modelling river water quality (Reichert et al., 2001). On the basis of these models, the IWA Task Group on River Water Quality Modelling has proposed the RWQM1 model for routine use. However, this model is rather complex and requires large input data sets. Therefore, a simplified version was derived during this study by selecting and modifying the most important sub-model components. The procedure for sub-model selection has been documented by Vanrolleghem et al (2001). The state variables and processes contained in the simplified version of the model are given in Table 1. The model components indicated in the Table 1 were selected based on the following simplifying assumptions:

- Only bacteria suspended in the water column were considered to dominate the conversion rates. Algae, macrophytes and consumers were assumed not to be relevant.
- Each river section was assumed to be completely mixed, and a one-dimensional model is considered. The sediment source and sink were not included in the model as separate compartments.
- CO_2, N_2, and H^+ were used to determine stoichiometric coefficients but were not included in the model as limiting factors, because they were considered always to be present in sufficient quantity.
- Nitrification was modeled as a single step ($X_{N1}+X_{N2}$ = X_N and $S_{NO2}+S_{NO3}$ = S_NO), and pH was assumed not to change significantly during the process.

TABLE 1 State variables and processes used in the simplified river quality model and relation to RWQM1 formulation (Reichert et al., 2001)

State variables	Description	Processes
S_I	Inert soluble COD	Aerobic growth of Heterotrophs with ammonia
S_S	Readily biodegradable COD	Aerobic growth of Heterotrophs with nitrate
S_O	Dissolved oxygen	Aerobic respiration of Heterotrophs
S_NH (S_{NH4}+S_{NH3})	Ammonia nitrogen	Anoxic growth of Heterotrophs with nitrate
S_NO (S_{NO2}+S_{NO3})	Nitrate+Nitrite nitrogen	Anoxic respiration of Hetrotrophs
S_PO (S_{HPO4}+S_{H2PO4})	Phosphate phosphorus	Growth of Nitrifiers
X_H	Heterotrophic biomass	Aerobic respiration of Nitrifiers
X_N (X_{N1}+X_{N2})	Nitrifying biomass	Hydrolysis of particulate organic materials
X_P	P adsorbed to particles	Adsorption of Phosphate
X_I	Particulate inert COD	Desorption of Phosphate
X_S	Particulate organic matter	

Stoichiometric coefficients were determined using a simple standard mass composition for organic substances considering the elements C, H, O, N and P. The conversion rates were all formulated with Monod-type limitation factors.

Using the WEST® modelling and simulation software (Hemmis NV, Kortrijk, Belgium), the complete tank in series model is illustrated in Figure 2.

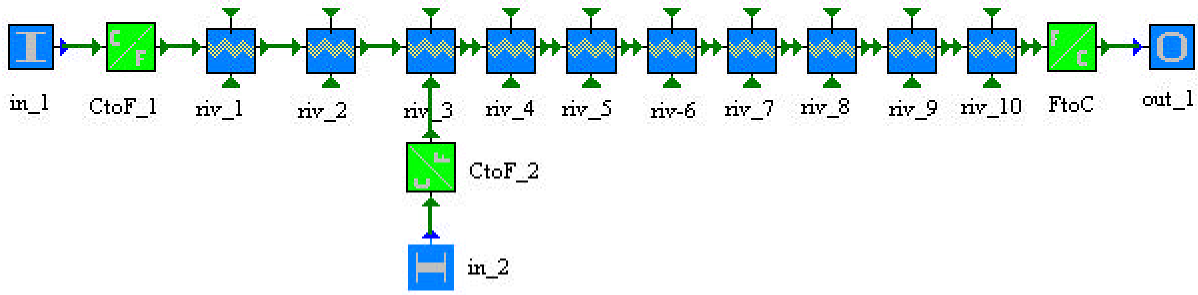

Figure 2. Diagram of the complete tank in series model, where: In_1 represents the input from upstream; In_2 is the input from the side river (Kaap River); boxes riv_1 to riv_10 describe continuously stirred tanks in series, and CtoF and FtoC boxes indicate concentration to flux and flux to concentration conversions sub-model respectively.

The approximate length and number of tanks in series for each river compartment (reach) are given in Table 2.

TABLE 2 River compartments

Reaches No.	Code of measurement stations (beginning – end)	Length (km)	Number of tanks in series	Cumulative distance from In_1 (km)
I	X2H006-X2H032	16	2	16
II	X2H032-X2H022	9	1	25
III	X2H022-X2H048	34	6	59
IV	X2H048-X2H046	11	1	70

The appropriate number of tanks in series was selected on the basis of the results obtained after several simulations with an increasing number of tanks while calibrating the model. The greater the number of tanks, the greater is the tendency towards ideal plug flow conditions. However, with progressively larger numbers of tanks, the calculation time also increases accordingly. Therefore, 10 tanks were considered to represent an acceptable compromise between calculation time and accurate representation of the river system.

MODEL CALIBRATION

The model was calibrated using a trial and error procedure. The number of tanks in series was selected based on the best curve fit with the measured data obtained after several simulations with an increasing number of tanks. Since the model also has considerable complexity and many parameters, the model was calibrated by tuning the most sensitive parameters in order to get the best curve fit with the measured data. The stoichiometric coefficients were calculated and the other parameters (yield coefficients and rate constants) were taken from literature (Reichert et al., 2001). The model was only calibrated by tuning the values for X_N and X_H in the upstream (in_1) and tributary inflows (in_2), with the assumption that the biomass density does not vary significantly. The values of these parameters were selected on the basis of best curve fitting with the measured data. The best curve fit was obtained with 0.1 X_N mg L^{-1} and 2 X_H mg L^{-1} with ten tanks in series.

RESULTS AND DISCUSSION

Since nutrient pollution is one of the main water quality problems in downstream sections of the Crocodile River, nitrogen pollution (nitrate nitrogen and ammonia nitrogen) formed the main focus of this study. The simplified model was used to predict nitrate and ammonia nitrogen concentrations in the downstream section of the Crocodile River. Based on two years (1989 to 1990) of monthly water quality data and daily flows at 4 measurement stations, the simulated results for nitrate and ammonia dynamics at the 16 and 70 km sites are illustrated in Figure 3 (a) and (b) respectively.

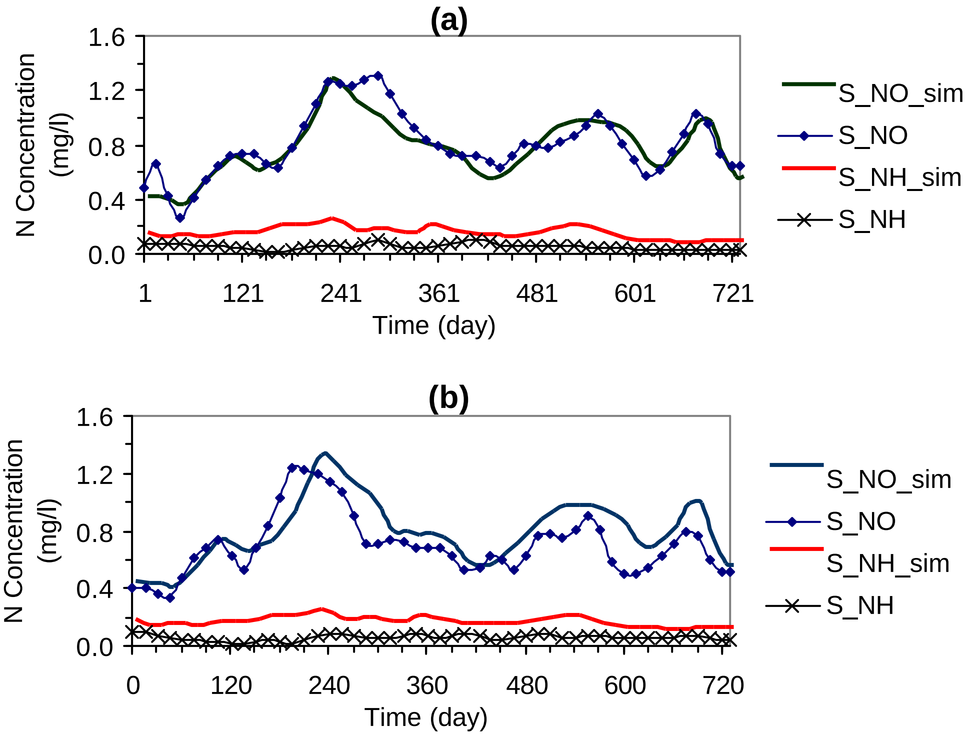

Figure 3. Comparison of measured and predicted nitrate (S_NO) and ammonia (S_NH) nitrogen dynamics at the downstream section of the Crocodile River (Jan 1, 1989 to December 31, 1990): (a) at the X2H032 sampling station (16 km); (b) at X2H046 sampling station (70 km).

As illustrated in Figure 3 (a) and (b), the simulated nitrogen concentrations (S_NO_sim and S_NH_sim) agree well with the measured data (S_NO and S_NH, respectively). The model prediction at the lower site (at 70 km) of the selected reach is better than for the upper part (16 km). The reason for this could be the lack of measured data on the domestic and industrial discharges in the intermediate upstream section (just after In_1). However, the simplified model adequately describes the general seasonal dynamics of nitrogen concentrations.

The seasonal variations in nitrogen concentration are inversely related to river flows, with higher nitrogen concentrations occurring during the dry season (July –September) when the river is at its minimum flow (Figure 4).

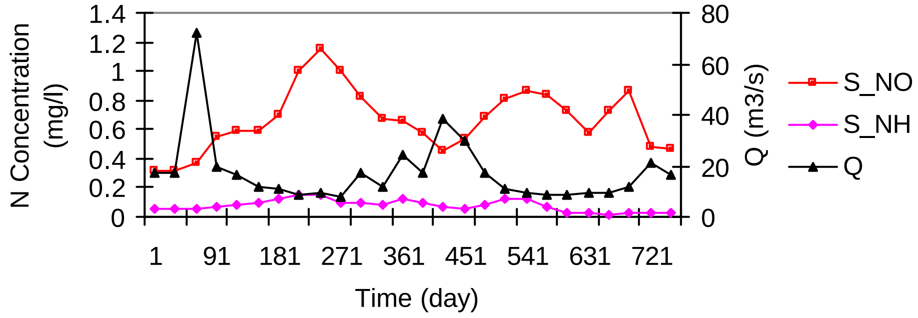

Figure 4. Comparison of river flow and nitrogen concentration dynamics at Crocodile-Kaap confluence (riv_3) in 1-Jan 89 to 31-Dec 90: S_NH is NH_4-N; S_ NO is NO_3-N, and Q is flow rate.

As the river flow increases the concentration of nitrogen decreases and vise versa (Figure 4). Normally, higher nutrient loads are washed from agricultural land into the river system during the wet season than during the dry season. However, nutrient concentrations remain low during the wet season because of the greater dilution. Accordingly, more attention should be given to the low dry weather river flows, with their associated higher nutrient concentrations, when modelling river water quality in the Crocodile River.

SENSITIVITY ANALYSIS

Parameter sensitivity in the simplified river water quality model, i.e. the response of an output variable such as nitrate or ammonia nitrogen to a change in single input variables, was required to gain an understanding of the likely model response to major input variables, and to provide a measure of the possible effect of uncertainty in the estimates of these variables on simulated nutrient concentrations.

Accordingly, the calculated concentrations of nitrate (S_NO) and ammonia (S_NH) were subjected to sensitivity analysis once the stoichiometric and kinetic parameters had been set using values obtained from the literature. The hydraulic parameters, and the concentrations of dissolved oxygen, nitrifiers and hetrotrophs in the model input were each increased by 10% to assess their influence on model performance.

In this study, relative sensitivities (S_R) were used to improve analysis. The relative sensitivity (relative-relative) measures the relative change of the model output in relation to a relative change of input variables. This choice is advantageous over absolute (absolute-absolute) sensitivities because it does not depend on the units of the parameters that are evaluated. The relative sensitivity (S_R) was calculated numerically, based on the change in predicted nitrogen concentration N upon a 10% increase of each parameter P:

$$S_R = \frac{\Delta N / N}{\Delta P / P} = \frac{\Delta N / N}{0.1.P / P} = 10.\frac{\Delta N}{N}$$

The sensitivity analysis results are presented in Table 3.

TABLE 3 Result of sensitivity analysis of simplified model: relative sensitivity (S_R)

	Parameter codes	Descriptions	S_R for Nitrate (%)	S_R for Ammonia (%)
1	X_N	Nitrifiers concentration	+6.62	-56.25
2	*ß*	Hydraulic parameter	+4.66	-36.13
3	*a*	Hydraulic parameter	-4.07	+30.88
4	T_max	Maximum water temperature	+3.16	-22.94
5	ET_max	Maximum ET	-0.31	+2.73
6	X_H	Hetrotrophs concentration	+0.16	+6.00
7	S_S	Readily biodegradable COD	-0.09	-0.35
8	S_O	Oxygen concentration	+0.04	-0.04
9	*v*	Flow velocity	+0.04	+0.01

As indicated in Table 3, the sensitivity of the predicted nitrate concentration to the parameters is as follows (ordered from most to least sensitive): concentration of X_N, *ß*, *a*, T_max, ET_max, X_H, S_S, S_O and *v*. The model sensitivity for ammonia is similar, except that the X_H concentration is placed fourth in the sequence of sensitive parameters. The sensitivity of both nitrate and ammonia to S_S, S_O and v is negligible and the uncertainty related to these parameters will therefore have less importance than the concentration of X_N. Even though the sensitivity of nitrate to ET is negligible, it is not negligible for ammonia because it determines the dilution rate. A higher ET value can result in higher ammonia concentration predictions. The nitrogen concentration also depends on the hydraulic parameters (*a* and *ß*) because these parameters determine the flow rates. Nitrogen predictions are also sensitive to T_max as the later determines the temperature dependent kinetic parameters (growth rate of nitrifiers and heterotrophs) and coefficients of chemical equilibria. In general, the relative sensitivity is higher for ammonia nitrogen than for nitrate nitrogen. This can be caused by the fact that some ammonia nitrogen is incorporated in new biomass rather than being completely transformed to nitrate nitrogen. Besides, ammonia nitrogen concentrations are very low when compared to nitrate nitrogen, which amplifies the relative sensitivity for ammonia.

CONCLUSIONS

Use of the simplified model reduced the data requirements significantly and the model can be applied for the Crocodile River. In its new configuration, the model is faster and requires less simulation time than the more complex original RWQM1. The model has sufficient complexity for description of short-term dynamics of ammonia and nitrate (periods spanning a few days to a few weeks). However, further analysis is required in order to investigate the potential importance of algae and its significance in different types of river systems. The demonstrated sensitivity of the model output to hydraulic parameters requires accurate parameter estimation based on flow and stage relations in every river reach. In addition, the concentration of nitrifiers should also be estimated carefully.

ACKNOWLEDGEMENT

The authors thank Belgium Technical Co-operation (BTC) for its financial support and Council for Scientific and Industrial Research (CSIR) in South Africa for providing Crocodile River water quality data.

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