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

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**Abstract.** The ultimate goal of this study is to develop a simple dynamic river water quality model that can be applicable in a data limited situation and is compatible with typical activated sludge models, so that the model can be used in integrated modelling of wastewater and river water quality in the future. A simplified river water quality model was formulated based on a conceptual hydraulic sub-model and simplification of an existing river water quality model. The simplified water quality was derived from the River Water Quality Model No. 1, which is one of the most comprehensive basic river water quality models available in literature. The applicability of the simplified model in data limited situations was investigated using a case study of inorganic nitrogen (nitrate and ammonia) in the Crocodile River (South Africa). The model was calibrated and validated on the basis of independent data collected for four years (1987–1990). The results show that the model can adequately describe the seasonal dynamics of inorganic nitrogen in the Crocodile River. The sensitivity of the model output to the model inputs was also analysed, and the results indicate that the model is most sensitive to the microbial biomass (nitrifier) followed by hydraulic parameters. The relation of river flow versus concentration of inorganic nitrogen in the downstream section of the river was also examined in order to identify the main source and critical time for nitrate pollution.

**Keywords:** ammonia, dynamic modelling, nitrate, river water quality, RWQM, sensitivity analysis

## 1. 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). 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 police and strategies towards integrated river basin approach require a mathematical model as a tool in water quality management (e.g. Tyson *et al*., 1993; Gu and Dong, 1998). While both monitoring and modelling provide important information for water quality regulator, water quality modelling is becoming increasingly important due to its unique predictive capabilities and its cost-effectiveness. It can be used for various scenario analyses and evaluation of

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alternative management operations to achieve water quality objective. Besides, the complex relationships between waste load from different sources (point or non-point) and the resulting water quality responses of the receiving waters are best described with mathematical models.

In literature, several types of basic river water quality models, which mainly deal with nutrient and oxygen balance, are available. The complexity and number of state variables of these models increase from the simplest Streeter-Phelps model, 'oxygen sag' (Streeter and Phelps, 1925) to extended models such as *QUAL1* (Orlob, 1982), *QUAL2* (Water Resource Engineering, 1973), *QUAL2E* (Brown and Barnwell, 1987), *MIKE11* (DHI, 1992), *DUFLOW-EUTROF1* (Aalderink *et al.*, 1995) and *ISIS* (Wallingford, 1996). Importantly, none of these models use microbial biomass as state variables despite the fact that microbial biomass determines the rates of biotransformation processes. Besides, the mass balance for carbonaceous organic matter is based on Biological Oxygen Demand (BOD). BOD-figures only represent a part of the biologically degradable matter, which makes it difficult to use BOD for the calculation of mass balances (Henze *et al.*, 1995a). They do not include the particulate organic matter, which is not bioavailable, and hence cannot be divided into different organic carbon fractions; the BOD-values are therefore not suitable to make a consistent mass balance.

Subsequently, the IWA river water quality task group proposed the River Water Quality Model No. 1 (RWQM1) (Reichert *et al.*, 2001). For consistency not only in mass balance but also in elemental balance, this model is based on Chemical Oxygen Demand (COD) as a measure of carbonaceous organic matter, similar to the Activated Sludge Models, ASM-1 (Henze *et al.*, 1987), ASM-2 (Henze *et al.*, 1995b) and ASM-3 (Gujer *et al.*, 1999). As such, it is compatible with the activated sludge models, and thus suitable for integrated water quality modelling of urban wastewaters and rivers (Meirlaen *et al.*, 2001). In RWQM1, COD values are divided into different organic fractions assuming constant elemental composition of compounds and organisms in the system. This allows using the mass fraction of elements (C, H, O, N and P) as model parameters. The stoichiometric coefficients of conversion processes are formulated as a function of these parameters. The rates of biochemical processes are formulated using Monod-type limitation factors.

However, RWQM1 is considered too comprehensive and complex to be applied directly in many situations where there are limited available data, which is the case in developing countries for instance. The model consists of 24 variables, 36 kinetic parameters, 6 equilibrium parameters, 13 stoichiometeric parameters, 36 mass fractions, and as such it requires a large input data set. The number of state variables and parameters becomes considerably larger when the benthic sediment is also included. It is also difficult to find sufficient and reliable data to calibrate these parameters. Thus, simplifying this model is necessary (Vanrolleghem *et al.*, 2001). In data poor situations, one needs to focus on a simple river water quality model that respects both mass and elemental balances and is still compatible with the activated sludge models.

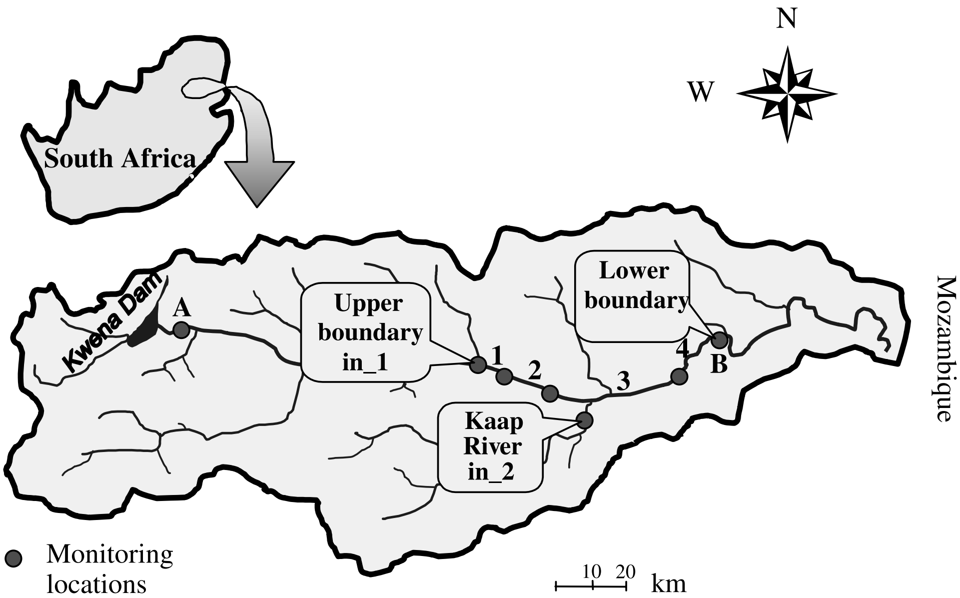


*Figure 1.* Crocodile River basin: the distance between two upper and lower boundaries (about 70 km) is the sensitive river section included in the model; in_1 (upstream point) and in_2 (Kaap River) are model inputs; 1 to 4 are main river segments.

The goal of this study is therefore to develop a simple dynamic river water quality model based on a conceptual hydraulic model and the simplification of the existing complex RWQM1 model (Reichert *et al.*, 2001). The usefulness of the model was evaluated based on a case study of inorganic nitrogen (ammonia and nitrate) concentrations in the Crocodile River, South Africa.

## 2. Material and Methods

### 2.1. 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 African largest and most important irrigation areas (DWAF, 1995; Van der Zel, 1977). 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. The total population residing in the catchment has been estimated to be 632 500 in the year 2005 (Ashton *et al.*, 1995), with approximately 76% of these residents located in urban areas. The Crocodile River is relatively a large river that 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.

The water quality of the Crocodile River 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, and mining sites (DWAF, 1995). 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 experience often serious water quality problems, particularly, the presence of toxic heavy metals, increased salinity and escalating eutrophication (DWAF, 1995).

For this study, a section of some 70 km of the downstream reaches of the Crocodile River (between marked upper boundary and lower boundary) (see Figure 1) was selected. The chosen river section represents the most sensitive portion of the river, where nitrate and ammonia concentrations often exceed the recommended maximum limits of 0.5 mg $L^{-1}$ (nitrate nitrogen) and 0.03 mg $L^{-1}$ (ammonia nitrogen) for oligotrophic systems (DWAF, 1993; Ashton *et al.*, 1995). The river also 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. In this river section, daily flows and monthly water quality data collected for several years are available. However, most of these data were collected in different time scales at different monitoring locations, and therefore they are not suitable for a dynamic water quality modelling. Only the data collected for four years (1987–1990) were used for this study.

### 2.2. MODEL FORMULATION

The content of this subsection will be discussed in two subsections. First the hydraulic sub-model formulation is presented. Second, the hydraulic model is extended to include the water quality sub-model (biochemical processes).

#### 2.2.1. *Hydraulics*

In the state-of-the-art, the complex hydrodynamic model that is based on typical St. Venant equations (De St. Venant, 1871) is applied in the river water quality studies like *ISIS, DUFLOW-EUTROF1*, and *MIKE11* and Salmon Q (Wallingford Software, 1994). Such complex hydrodynamic model is needed when there is backwater effect of weirs or other hydraulic controls like tidal effect. However, the application of such complex hydrodynamic model requires long computation time, and therefore not suitable for water quality studies like sensitivity analysis and parameter optimisation. In the absence of tidal effect, such complex hydraulic model can therefore be simplified into a conceptual hydraulic model in which the river is represented as a Continuously Stirred Tank Reactor in Series (CSTRS) (Whitehead *et al*., 1979; Beck and Reda, 1994). Using CSTRS as a surrogate for the complex hydrodynamic model, the water balance equation in a single tank can be expressed as follows:

$$\frac{dV}{dt} = Q_{in} - Q_e - ET \cdot A \ , \tag{1}$$

where $V$ is the volume of the tank ($L^3$); $Q_{in}$ is the influent flow rate to the tank [$L^3$ $T^{-1}$]; $Q_e$ is the effluent flow rate from the tank [$L^3$ $T^{-1}$]; *ET* is evapotranspiration [L $T^{-1}$]; and $A$ is the surface area of the river tank [$L^2$].

In arid and semi-arid regions, the inclusion of an evapotranspiration factor (*ET*) in the model is very important, particularly when dealing with the Crocodile River where the annual mean of potential evapotranspiration loss for the catchment (1800–2000 mm) exceeds the mean annual precipitation (<800 mm) by a wide margin (DWAF, 1995). Because considerable water loss by evapotranspiration can results in an increase of the concentration of constituents in the river, the impact on the river water quality should not be neglected. Salinity, for example, is one of the adverse consequences in downstream reaches of the catchment. Obviously, such problem can be exacerbated by human activities such as irrigation and mining. On the basis of data collected in July 1990, the values of Electrical Conductivity (EC) as a measure of salinity increases with river length (from about 13 mS $m^{-1}$ at 14 km (mark A) to 40 mS $m^{-1}$ at a distance of 270 km (mark B) from the Kwena Dam (see Figure 1).

The effluent flow rate and flow longitudinal flow velocity in each 'river tank' can be calculated as follows:

$$Q_e(t) = \alpha h(t)^{\beta} \tag{2}$$

$$v(t) = \frac{Q_e(t)}{A_{\text{cross}}} \ , \tag{3}$$

where $h(t)$ is the hydraulic depth at time $t$ [L] = $V(t)/A_{\text{surface}}$; $\alpha$ and $\beta$ are the hydraulic parameters estimated from stage flow relations; $v(t)$ is the flow velocity at time $t$ [$LT^{-1}$]; $A_{\text{surface}}$ is the top surface area at time $t$ [$L^2$]; and $A_{\text{cross}}(t)$ is the cross sectional area at time $t$ [$L^2$].

For simplicity, $A_{\text{surface}}$ was calculated based on a rectangular channel approximation. It is not clear whether this approximation is justifiable for rivers, which are slow flowing and meandering. However, it is indicated in literature that when the river flow width is significantly larger than the flow depth (5 to 10, depending on the roughness or meandering), it can be assumed as a rectangular cross-section (Chow, 1981). According to Chow, a wide-open channel can safely be defined as a rectangular channel when the flow width is 10 times the flow depth. In the studied river section, in most of the cases, the flow width is greater than 10 times the flow depth, and therefore a rectangular channel approximation appears justified.

TABLE I

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

| | State variables | Description |
|---|---|---|
| 1 | *S_I* | Inert soluble COD |
| 2 | *S_S* | Readily biodegradable COD |
| 3 | *S_O* | Dissolved oxygen |
| 4 | *S_NH* $(S_{NH_4} + S_{NH_3})$ | Ammonia nitrogen |
| 5 | *S_NO* $(S_{NO_2} + S_{NO_3})$ | Nitrite + Nitrate nitrogen |
| 6 | *S_PO* $(S_{HPO_4} + S_{H_2PO_4})$ | Phosphate phosphorus |
| 7 | *X_H* | Heterotrophic biomass |
| 8 | *X_N* $(X_{N1} + X_{N2})$ | Nitrifying biomass |
| 9 | *X_P* | P adsorbed to particles |
| 10 | *X_I* | Particulate inert COD |
| 11 | *X_S* | Particulate organic matter |

2.2.2. *Water quality*

The above relatively simple hydraulic model equation (1) can then be extended to include the water quality sub-model. The general mass balance for the reactive water quality constituents in every river tanks of CSTRS is expressed as follows:

$$\frac{d(VC)}{dt} = Q_{in}C_{in} - Q_e C + Vr \ , \tag{4}$$

where $C_{in}$ is the influent concentration [ML$^{-3}$]; $C$ effluent concentration [ML$^{-3}$]; $r$ reaction rate [ML$^{-3}$ T$^{-1}$].

During this study, another mass balance equation was derived based on Equations (1) and (4) as follows:

$$\frac{dC}{dt} = \frac{Q_{in}}{V}C_{in} - \frac{1}{V}\left(Q_{in} - ET{*}A\right) C + r \ . \tag{5}$$

Equation (6) shows that 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 can be calculated with the same equation as for a tank with constant volume, but now a time dependent volume is used. Such model formulation however requires the hydraulics calculations to be performed separately and prior to the calculation of the mass balance.

The conversion process ($r$) in Equations (4) and (5) describes changes in water quality components due to biological, chemical and physical processes. To model

TABLE II

Processes used in the simplified river water quality model and relation to RWQM1 formulation (Reichert *et al.*, 2001)

| | |
|---|---|
| 1 | Aerobic growth of Heterotrophs with ammonia |
| 2 | Aerobic growth of Heterotrophs with nitrate |
| 3 | Aerobic respiration of Heterotrophs |
| 4 | Anoxic growth of Heterotrophs with nitrate |
| 5 | Anoxic respiration of Heterotrophs |
| 6 | Growth of Nitrifiers |
| 7 | Aerobic respiration of Nitrifiers |
| 8 | Hydrolysis of particulate organic materials |
| 9 | Adsorption of Phosphate |
| 10 | Desorption of Phosphate |

these conversion processes, a simplified version of RWQM1 (Reichert *et al.*, 2001) was applied. This was done using the general steps given in (Vanrolleghem *et al.*, 2001). The state variables and processes contained in the simplified version of the model are given in Tables I and II, respectively, based on the following simplifying assumptions:

- Only microbial biomass suspended in the water column were considered to dominate the conversion rates. Algae macrophytes (rooted or floating water hyacints) and consumers were assumed not to be relevant in the present work. It is possible to include them in the model, but there are no monitoring data to calibrate or validate the model.
- $CO_2$, $N_2$, 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 modelled as a single step (first step nitrifiers ($X_{N1}$) + second step nitrifiers ($X_{N2}$) = Nitrifying biomass (*X_N*); and nitrite nitrogen ($S_{NO_2}$) + nitrate nitrogen ($S_{NO_3}$) = *S_NO*).
- The pH was assumed not to change significantly during the process, thus the pH dependent state variables and related processes such as chemical equilibria can be omitted.

### 2.3. Model implementation

The proposed model was implemented in the WEST® simulator (Vanhooren *et al.*, 2002), which has been applied mainly to wastewater treatment plant systems, but can also be applied readily to river water quality systems by extending the open

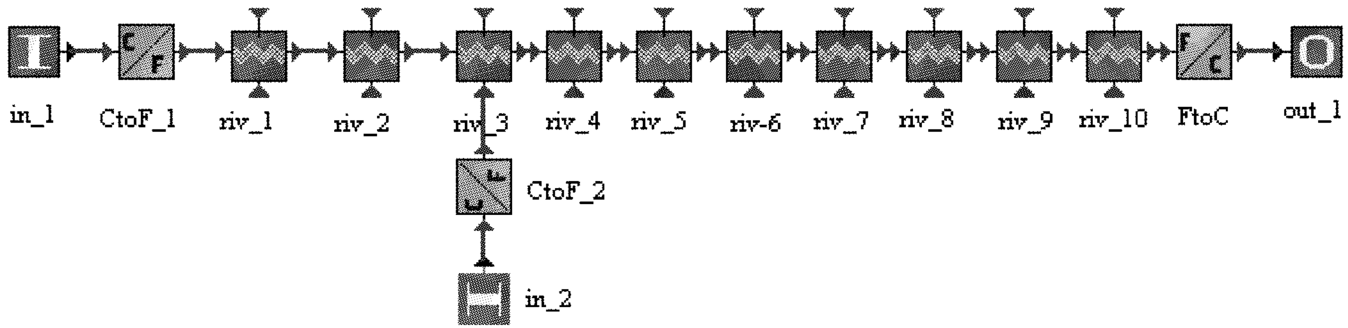


*Figure 2.* Diagram of the complete tank in series model, where: in_1 represents the input from upstream; in_2 is the input from the side river (Kaap River); boxes riv_1 to riv_10 describe continuously stirred tanks in series, and CtoF and FtoC boxes indicate concentration to flux and flux to concentration conversions sub-models, respectively; out_1 is the output at the lower boundary.

‘modelbase’. For the selected section of the Crocodile River (see Figure 1), the complete CSTRS model configuration in the WEST® simulator is illustrated in Figure 2.

In Figure 2, only two inputs (in_1 and in_2) were considered in the selected river section because there was no additional quantitative information related to wastewater effluent discharges available.

### 2.4. Model calibration and validation

The model was calibrated and validated on the basis of independent data set. The calibration was done in two steps. In the first step, the hydraulic parameters ($\alpha$ and $\beta$) were estimated on the basis of flow-stage relationships at the two monitoring locations (16 and 70 km) of the study section of the river. In the second step, an appropriate number of tanks in series was selected on the basis of a best curve fit (root mean square error) obtained after several simulations with an increasing number of tanks. However, with progressively larger numbers of tanks, the calculation time also increases accordingly. The optimum number of tanks in series was then selected based on a compromise between model fit and simulation time.

In the second step, the water quality sub-model was calibrated by changing the most influential water quality parameters (based on the sensitivity analysis) until the best agreement between the measured and the simulated data set was obtained. As the available water quality data are not sufficient to calibrate all water quality parameters, only few parameters such as the concentrations of *X_N* and *X_H* in the upstream (in_1) and in the side stream inflow (in_2) were calibrated with the assumption that the biomass density does not vary significantly. In this assumption, *X_H* and *X_N* are considered as model parameters (constants), despite the fact that they should be state variables and need to be monitored or estimated at every monitoring location. However such simplification of the model is very useful when not enough information for dynamic modelling of their population in the inputs is available (Vanrolleghem *et al.*, 2001). The stoichiometric coefficients were calculated based on the simplified processes rates given in Table II, and the other parameters (yield coefficients and rate constants) were taken from literature (Reichert *et al.*, 2001).

The simplified model was then validated on the basis of independent data collected in 1989 and 1990. The model was run with this independent data set without changing the calibrated parameters, and the simulated data set was then compared with the measured data set. The results were then evaluated based on the curve fit.

### 2.5. Sensitivity analysis

This insight was required to gain better understanding of the likely model response to a small change of major input variables, and to provide a measure of the possible effect of uncertainty in the estimates of these variables on simulated nutrient concentrations.

TABLE III
River segmentation

| Segment No. | Length (km) | Number of CSTRS | Cumulative distance from in_1 (km) | Hydraulic parameters | | |
|---|---|---|---|---|---|---|
| | | | | $\alpha$ | $\beta$ | $R^2$ |
| 1 (riv_1 - riv_2) | 16 | 2 | 16 | 27.29 | 1.527 | 0.996 |
| 2 (riv_3) | 9 | 1 | 25 | 119.85 | 1.502 | 0.951 |
| 3 (riv_4 – riv_9) | 34 | 6 | 59 | 365.60 | 1.721 | 0.977 |
| 4 (riv_10) | 11 | 1 | 70 | 21.26 | 3.267 | 0.857 |

In this study, a relative sensitivity function ($S_R$) (relative-relative) was used which measures the relative change of the model output in relation to a relative change of input variables or parameters. 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 $P$ at each simulation time step:

$$S_R(t) = \frac{\frac{\Delta N}{N(t)}}{\frac{\Delta P}{P}} = \frac{\frac{\Delta N}{N(t)}}{0.1\frac{P}{P}} = 10\frac{\Delta N}{N(t)} . \tag{6}$$

The values of the sensitivity function in Equation (6) are time dependent, which is the case for any dynamic simulation. Thus, the average absolute values of $S_R$ ($|\bar{S_R}|$) were used to rank the relative importance of the parameters (see Table III).

## 3. Results and Discussion

### 3.1. Model calibration

Ten CSTRS were considered to represent an acceptable compromise between calculation time and accurate representation of the river system. In high temporal resolution e.g. less than an hourly basis, ten STRS may be a crude assumption for a 70 km river stretch, and it would then certainly need a tracer study to determine the optimum number of STRS. In this study, using a higher number of CSTRS (e.g. twenty tanks) did not improve the model prediction (rather it increased the simulation time by more than two times). As the simulation time is important, ten CSTRS were considered as a rough representation of dispersion of the river.

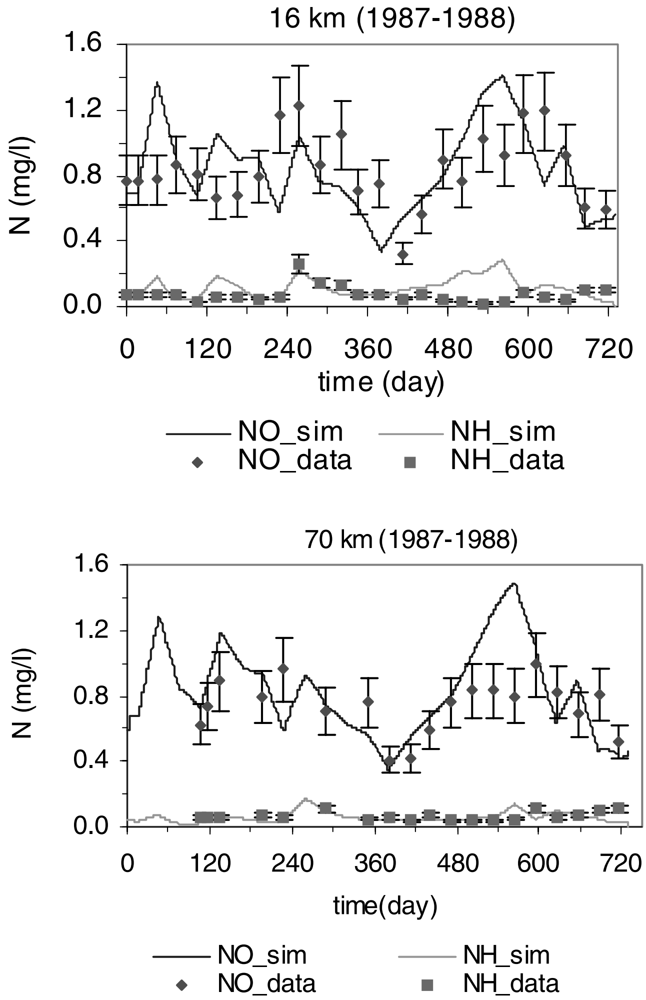


*Figure 3.* Model calibration: comparison of measured nitrate (S_NO_data) and ammonia (S_NH_data) nitrogen versus simulated nitrate (S_NO_sim) and ammonia (S_NH_sim) nitrogen concentration.

The approximate length and number of tanks in series for each river reach (segment) indicated in Figure 2 are given in Table III. The hydraulic parameters $\alpha$ and $\beta$ were determined using flow- stage relationship at monitoring locations of 16 and 70 km (see Table III). Between these two locations, the values were obtained by calibration.

The model was calibrated based on monthly water quality and daily flow data collected in 1987 and 1988 at two monitoring locations (at 16 and 70 km) (see Figure 3). The results indicate that the general trend of simulated nitrogen concentrations (for both nitrate and ammonia) agree well with measured data within 20% error. In some points, there are indeed some differences between the measured and

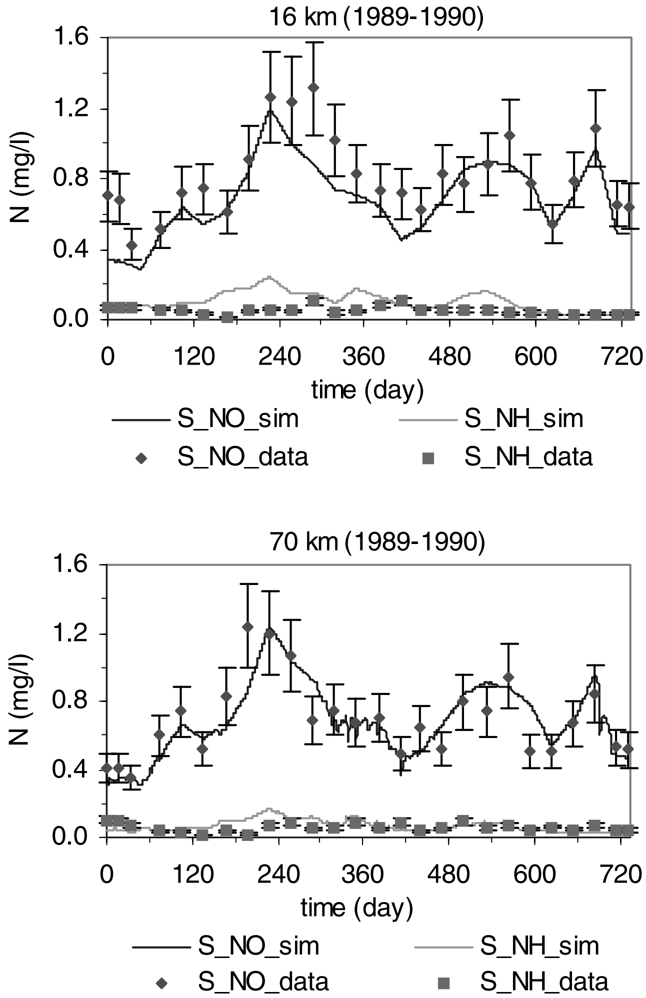


*Figure 4.* Model validation: comparison of measured nitrate (S_NO_data) and ammonia (S_NH_data) nitrogen versus simulated nitrate (S_NO_sim) and ammonia (S_NH_sim) nitrogen concentration.

simulated data sets. This difference could be because monthly water quality data are based on the collection of point measurements (once per month), which do not represent the average monthly water quality data. Besides, for the continuous measurement required in the model inputs (in_1 and in_2), the daily water quality data were linearly interpolated from the point measurements of monthly water quality data. In spite of the differences between measured (data) and simulated (sim) data sets, the calibration results are quite acceptable.

TABLE IV

Result of sensitivity analysis of simplified model: relative sensitivity ($S_R$)

| | Parameter codes | Descriptions | $\lvert \bar{S_R} \rvert$ for Nitrate (%) | $\lvert \bar{S_R} \rvert$ for Ammonia (%) |
|---|---|---|---|---|
| 1 | *X_N* | Nitrifiers concentration | 6.62 | 56.25 |
| 2 | $\beta$ | Hydraulic parameter | 4.66 | 36.13 |
| 3 | $\alpha$ | 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* | Heterotrophs 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 |

### 3.2. Model validation

To validate the model, the calibrated model was run with new independent data collected in 1989 and 1990 without changing the calibrated model parameters. Figure 4 shows the results. For both ammonia and nitrate nitrogen concentrations at the two monitoring stations (16 and 70 km), the predicted data set agree well with measured data set (within 20% error, like the calibration results).

The result is quite reasonable for such limited data. When a higher accuracy of the model is desired, a higher measurement frequency will be required e.g. daily or sub-daily (instead of monthly, which is the case in this study) at every monitoring location in the main river and in all its side streams or tributaries. Obviously, such higher frequency of data collection is not always feasible, especially in developing countries where the available financial resources are often limited to make the required monitoring campaign. Nevertheless, by using the proposed simplified model the data requirement can be reduced significantly.

### 3.3. Sensitivity analysis

The sensitivity of the model output (the concentrations *S_NO* and *S_NH*) to the model input was analysed. The model input was increased by 10%, and the average absolute values of relative sensitivity of the predicted concentrations of *S_NO* and *S_NH* were calculated (see Table IV). The sensitivity of the predicted nitrate concentration to the model inputs is as follows (ordered from most to least sensitive): concentration of *X_N*, $\beta$, $\alpha$, *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 the predicted

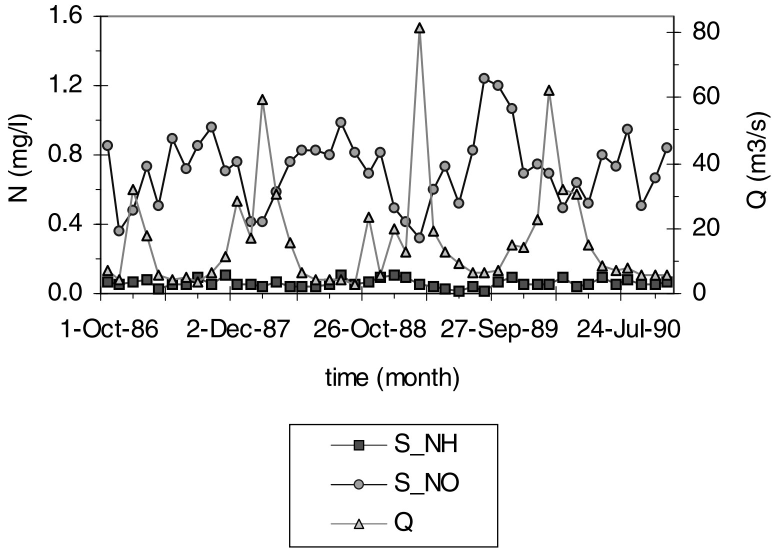


*Figure 5.* River flows versus inorganic nitrogen-concentrations at 50 km, $Q$ is the flow rate.

concentration of both nitrate and ammonia nitrogen 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_max* is negligible, it is not negligible for ammonia because it determines the dilution rate. A higher *ET_max* can result in higher ammonia concentration predictions. The nitrogen concentration prediction also is relatively very sensitive to the hydraulic parameters ($\alpha$ and $\beta$) 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).

In general, the relative sensitivity is higher for ammonia nitrogen than for nitrate nitrogen. The main reason is the fact that ammonia nitrogen concentrations are relatively very low when compared to nitrate nitrogen. Such low ammonia concentration thus amplifies the relative sensitivity for ammonia because the resulting change in simulated ammonia concentration has to be divided by a relatively small value of ammonia concentration as compared to the nitrate nitrogen (see also Equation (6)).

### 3.4. River flow versus nitrogen concentration

Using data collected in 1986 to 1990, the relationship between river flow versus inorganic nitrogen concentration in the down stream section of the river (at 50 km) was analysed. The results show that the concentration of nitrogen is inversely related to the river flow (see Figure 5). The higher nitrogen concentrations occur during the dry season when the river is at its minimum flow. As the river flow increases the concentration of nitrogen decreases and vice versa. Therefore, low flow periods (dry season) are the worst case for nitrate and ammonia.

Furthermore, one may expect higher nitrogen concentrations during the wet season than during the dry season because of the higher nitrogen load washed from agricultural land or mining sites into the river system during the wet season. This is true when the contribution from non-point source (diffused source) is higher than from point sources or side streams (Behrendt, 1993). In the studied section of the Crocodile River however, the concentrations of inorganic nitrogen (or better, nitrate nitrogen) remain low during high flows because of the greater dilution, and vice versa. Such inverse relationship between the concentrations of inorganic nitrogen and river flows in a downstream point of the study section shows that the main sources of inorganic nitrogen are side streams (point sources). The main contribution is from the Kaap River (in_2), which drains an extensive area of active and abandoned gold mines. This has resulted in poor water quality of the river in the downstream sections from the Crocodile-Kaap River confluence (Kleynhans, 1999). In the water quality management of the Crocodile River, more attention should therefore be given to the low flow period when the main river flow might be too low to dilute the Kaap River and to flush possible wastewater effluent discharges.

### 3.5. Model application and data requirement

The data requirement of the proposed model is determined by the application of the model. If the seasonal dynamics of the water quality variables is of interest, monthly water quality data can be used like in this study. If the monthly water quality data are based on point measurements (measuring once a month), reliability may be doubted as this is influenced by inherent variation of runoff events or river flows. As the model is designed for short-term river water quality studies, the more frequent the monitoring data are collected (e.g. weekly to daily, depending on the available financial and material resources) the better will be the model accuracy in describing the dynamics of nutrients in the river. To apply this model on a daily basis the following minimum data are required: physical and hydraulics characteristic of the river, dissolved and particulate organic matter, dissolved oxygen, inorganic nitrogen, (nitrate + nitrite) and (ammonia + ammonium), water temperature and phosphate phosphorus.

## 4. Conclusions

A dynamic simplified river water quality model that can simulate the seasonal dynamics of inorganic nitrogen (ammonia and nitrate) in the Crocodile River was presented. The sensitivity of the model output to the model input or parameters was analysed. The relationship between river flow and nitrogen dynamics was also examined. Based on the results obtained during this study, one can draw the following general conclusions:

- Use of the simplified model reduced the data requirements significantly, and the model can be applied to the Crocodile River with limited available data.
- In its new configuration, the model is faster and requires less simulation time than the more complex original RWQM1.
- In the downstream section of the Crocodile-Kaap confluence, low flow periods were the worst case for ammonia and nitrate pollution as a result of the polluted side stream Kaap River (as a point source).
- The demonstrated sensitivity of the model output to the model inputs and parameters makes that accurate estimation of these parameters is required; particularly the hydraulic parameters need to be estimated using flow and stage relations in every river reach.
- The concentration of nitrifiers is the most sensitive parameter, and its appropriate estimation is important.
- The model has sufficient complexity for description of short-term dynamics of ammonia and nitrate (periods spanning a few days to a few weeks depending on the availability of data).
- In general, this study therefore demonstrated the usefulness of model reduction (model simplification) for the application of an appropriate but very complex river water quality model (like RWQM1) with minimum data requirements.

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