

Modelling nitrogen dynamics in an agricultural-forested catchment

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Abstract A spatially distributed nitrogen simulation (DNS) model has been developed to simulate daily nitrogen concentration variation in an agricultural-forested catchment. The model can simulate hydrological processes and various nitrogen processes at the grid cell level, continuously considering plant uptake, atmospheric wet deposition, fertilizer application, mineralization, nitrification and denitrification. The hydrological component is based on the distributed Xinanjiang (DXAJ) rainfall-runoff model, and the nitrogen component simulates key sources and sinks using a series of first-order kinetic equations. In particular, plant growth indices for land-use classes are incorporated to simulate plant uptake variation in accordance with seasonal vegetation cover variations. Model calibrations showed that there is a reasonable agreement between simulated and observed stream nitrate-nitrogen concentration. Sensitivity analysis showed that plant uptake is the key nitrogen sink, whereas agricultural fertilizer application is the key source of nitrogen.

Key words kinetic equations; nonpoint source; nitrogen modelling; plant uptake; Xinanjiang model

INTRODUCTION

Nitrogen levels in a river system reflect the integration of a number of sources within the catchment including nonpoint sources, such as agricultural fertilizer input and atmospheric deposition, and/or point sources such as domestic and industrial discharges. Superimposed on these anthropogenic contributions are “natural” contributions from the mineralization and nitrification of organic nitrogen in soils (Whitehead *et al.*, 1998a; Wade *et al.*, 2001). Climatic and seasonal factors (e.g. drought, temperature), and a number of land-use and management practices will influence various nitrogen species, such as nitrate-N and ammonium-N. The nitrogen profile of a river will thus be a unique function of regional climate and catchment characteristics such as land use, urbanization, short- and long-range deposition from emission sources, topography and hydrology (Whitehead *et al.*, 1998a).

The objective of this study is to develop a simple process-based nitrogen simulation component which can be coupled onto a distributed hydrological model to simulate nitrogen dynamics, considering key nitrogen processes and particularly, seasonal vegetation cover variations in the catchment.

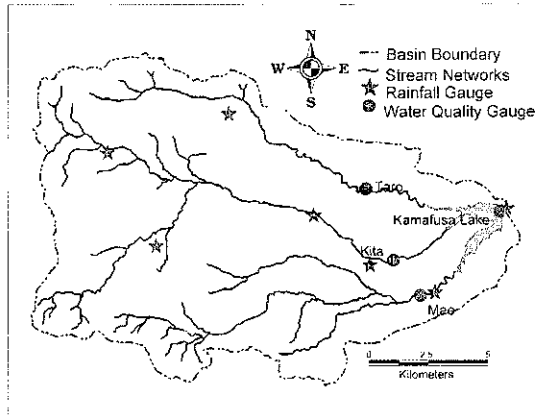


Fig. 1 Study area: the Kamafusa Lake catchment

STUDY AREA

The study area, the Kamafusa Dam catchment, is located at Kawasaki Town ($140^{\circ}27'39''$ – $140^{\circ}43'05''$ E, $38^{\circ}15'56''$ – $38^{\circ}07'22''$ N), in the Miyagi Prefecture of Japan (Fig. 1). It is a mountainous agricultural-forested catchment with a catchment area of 195.2 km^2 ; its elevation ranges from 144 m at the lake to 1480 m in the mountainous area. There are three main tributaries, the Mae, Kita and Taro rivers, which flow to the Kamafusa Lake separately. The catchment includes about 82, 11 and 2% of forest, agricultural area and residential area, respectively.

DISTRIBUTED XINANJIANG MODEL

The original Xinanjiang (XAJ) rainfall–runoff model is one kind of semi-distributed model, in which the whole catchment area is divided into several sub-areas according to the Thiessen method, and runoff generation in each sub-area is simulated and routed to the catchment outlet using the Muskingum method.

In order to establish the distributed version of the Xinanjiang model, known as the distributed Xinanjiang (DXAJ) model, a distributed routing scheme is necessary. In the DXAJ model, the whole catchment is divided into grid cells (in this case $50 \times 50 \text{ m}^2$, which corresponds the available DEM resolution), and the runoff generation and separation components of the original Xinanjiang model are used to generate runoff in each grid cell and separate it into two water components: direct runoff and sub-surface runoff (baseflow). An optimal routing order approach (Lu *et al.*, 1993, 1996a,b) is applied to fulfil the distributed routing with the aid of a kinematic wave approximation. In order to determine the optimal routing order for the study area, the delineation of artificial stream networks is done using the Jenson & Domingue (1988) algorithm, which includes the calculation of flow directions and accumulations (Fig. 2). This optimal routing order, which is represented in a sequential file (Table 1) and includes several hydraulic attributes necessary for distributed routing, controls the sequences of distributed calculation from upstream channel to downstream, grid cell

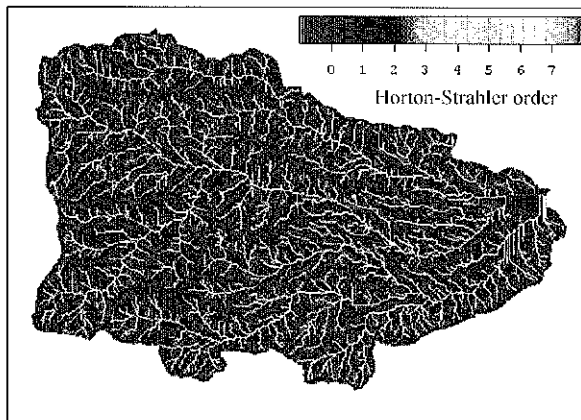


Fig. 2 Delineated stream networks (shown by Horton-Strahler order).

Table 1 Part of optimal routing sequential file used in DXAJ model.

Record no.	line ^a	col ^a	bin ^b	bout ^b	Slope ^c	Length ^d (m)	Flow ^e accum.	Elev. ^f (m)	LU code ^g
1	115	64	0	1	0.502	57.8	1	953	5
2	114	64	1	1	0.355	53.5	2	924	5
3	113	64	1	1	0.371	53.8	3	905	5
26529	153	255	2	2	0.009	50.0	26529	238	2
26530	156	256	0	7	0.099	50.3	1	249	2
75847	146	416	8	8	0.020	50.0	75847	144	20

^a location in line and column; ^b input buffer and output buffer; ^c slope of simulated channel; ^d length of the simulated channel; ^e flow accumulation; ^f elevation; ^g land use code, including: 1 paddy field, 2 cropland, 3 fruit tree, 4 other plants, 5 forest, 6 barren land, 7 residential area, 9 land used for traffic, 10 other land uses, 20 inland water.

by grid cell. The number of input buffer (bin) and output buffer (bout) of each channel are equal to the stream order of the channel, and the stream order of the output channel, respectively. More details of this approach can be referred to in Lu *et al.* (1993, 1996a,b).

In the DNS model, the distributed Xinanjiang (DXAJ) model is applied as a fundamental component, onto which an algorithm of key nitrogen processes is coupled to simulate the daily nitrogen dynamics. Rainfall input is distributed to each grid cell using distance-weighted rainfall, and evapotranspiration is estimated using the Hamon equation (JSCE, 1999) and adjusted to each grid cell allowing for air temperature variation depending on elevation.

NITROGEN PROCESSES AND EQUATIONS

Nitrogen processes in the catchment

The basic mathematical model for nitrogen dynamics in a catchment is assumed to have the following general form, in which nitrogen sinks and sources are aggregated (Nielsen *et al.*, 1978a,b):

$$\frac{d[N_c]}{dt} = -\sum_{i=1}^n k_i [N_c] + \sum_{j=1}^m k_j [N_m] \quad (1)$$

where N_c is the concentration of nitrogen species of interest and N_m is the concentration of other nitrogen species, k_i and k_j are the respective first-order kinetic rate constants for $i = 1 \dots n$ sink, and $j = 1 \dots m$ source mechanisms, and t is time.

In the DNS model, equation (1) is applied to each grid cell together with the distributed Xinanjiang (DXAJ) model to simulate daily hydrological processes and nitrogen dynamics in this grid cell, and the generated nitrogen load (flux) is transported together with runoff to the downstream grid cell, using a distributed routing approach. In practice, nitrate-N and ammonium-N species are assumed to be entrained and concentrate into surface and sub-surface water fluxes, and once in the artificial stream networks are routed to downstream conservatively. The key processes are described by:

$$\text{Nitrate-N: } \frac{d[\text{NO}_3^-]}{dt} = C_1 + C_2 + k_1[\text{NH}_4^+] - (k_2 + k_3)[\text{NO}_3^-] \quad (2)$$

$$\text{Ammonium-N: } \frac{d[\text{NH}_4^+]}{dt} = C_3 + k_6[\text{NH}_4^+] - (k_1 + k_4 + k_5)[\text{NH}_4^+] \quad (3)$$

where positive or negative terms represent sources or sinks of specific N species respectively. C_1 or C_3 is the input rate of NO_3^- or NH_4^+ , which can be calculated from wet deposition, fertilizer input and domestic sources. C_2 is non-biological N fixation rate ($\text{g m}^{-3} \text{day}^{-1}$). Parameters k_i ($i = 1, \dots, 6$) are the kinetic rate constants (day^{-1}) for first order nitrogen kinetic processes of nitrification (conversion from NH_4^+ to NO_3^-), plant uptake of nitrate-N, denitrification (conversion from NO_3^- to gaseous N_2O , N_2 , etc.), plant uptake of ammonium-N, immobilization (NH_4^+ fixation by microbes) and mineralization (conversion from organic N to NH_4^+). All parameters used in the DNS model are described in Table 2.

Kinetic rate constants

The kinetic rate constants (day^{-1}) are soil temperature-dependent using the following equation (Whitehead *et al.*, 1998a,b, 2002; Collins *et al.*, 1999; Wade *et al.*, 2001):

$$k_i = k_{i(20^\circ\text{C})} 1.047^{(ST-20)} \quad (4)$$

where $k_{i(20^\circ\text{C})}$ ($i = 1, \dots, 6$) are the corresponding kinetic rate constants at soil temperature of 20°C . Soil temperature (ST) is estimated from a seasonal relationship dependent on daily average air temperature as following:

$$ST = T_{air} + C_5 \sin\left(\frac{3}{2}\pi \frac{DOY}{365}\right) \quad (5)$$

where T_{air} is the daily catchment average air temperature and DOY is the day number of a year.

Table 2 Model parameters of three main land-use types (at soil temperature of 20°C).

	Definition of parameters	Forest	Agricultural	Residential
k_1	Ammonium nitrification rate constant (day^{-1}) ^a	0.100	0.100	0.000
k_2	Plant uptake rate constant of $[\text{NO}_3^-]$ (day^{-1}) ^a	0.850	0.500	0.000
k_3	Denitrification rate constant (day^{-1}) ^a	0.500	0.100	0.000
k_4	Plant uptake rate constant of $[\text{NH}_4^+]$ (day^{-1}) ^a	0.100	0.120	0.000
k_5	Ammonium immobilization rate constant (day^{-1}) ^a	0.100	0.100	0.000
C_2	Nitrogen fixation rate ($\text{g m}^{-3} \text{day}^{-1}$) ^b	0.002	0.002	0.000
k_6	Ammonium mineralization rate constant (day^{-1}) ^a	0.080	0.140	0.000
C_5	Maximum temperature difference (air–soil) ($^{\circ}\text{C}$) ^b	4.500	4.500	0.000
C_7	Plant growth start day (DOY)	110.00	128.00	0.000
C_{10}	Daily average $[\text{NO}_3^-]$ concentration of rainwater (g m^{-3}) ^c	0.100	0.100	0.100
C_{11}	Daily average $[\text{NH}_4^+]$ concentration of rainwater (g m^{-3}) ^c	0.050	0.050	0.050
C_{13}	Ammonium-N (fertilizer) addition rate ($\text{kg N ha}^{-1} \text{year}^{-1}$)	0.000	40.000	0.000
C_{14}	Nitrate-N (fertilizer) addition rate ($\text{kg N ha}^{-1} \text{year}^{-1}$)	0.000	40.000	0.000
C_{15}	Fertilizer addition period (days)	0.000	130.000	0.000
C_{16}	Fertilizer addition start day (DOY)	0.000	120.000	0.000
C_{18}	Coefficient for calculating plant growth index	0.681	0.719	0.000
C_{19}	Coefficient for calculating plant growth index	0.143	0.174	0.000
C_{20}	Soil moisture threshold (mm)	60.00	60.00	0.000
C_{21}	Daily average domestic $[\text{NO}_3^-]$ discharge rate ($\text{g day}^{-1} \text{capita}^{-1}$)	0.000	0.000	6.800
C_{22}	Daily average domestic $[\text{NH}_4^+]$ discharge rate ($\text{g day}^{-1} \text{capita}^{-1}$)	0.000	0.000	3.500
C_{23}	Population density on residential area (capita ha^{-1})	0.000	0.000	3.14

^a Calibrated; ^b after Whitehead *et al.* (1998b); ^c Tabuchi *et al.* (1985). Others are specific to the study area.

Plant uptake

Plant uptake varies according to land use in terms of both the rate of uptake and the seasonal variation of uptake. The following equations are used to estimate the plant uptake of nitrate-N or ammonium-N:

$$Uptake_{[\text{NO}_3^-]} = k_2 C_6 [\text{NO}_3^-] \quad (6a)$$

$$Uptake_{[\text{NH}_4^+]} = k_4 C_6 [\text{NH}_4^+] \quad (6b)$$

where C_6 is seasonal plant growth index (Hall *et al.*, 1993) as:

$$C_6 = C_{18} + C_{19} \sin\left(2\pi \frac{\text{DOY} - C_7}{365}\right) \quad (7)$$

C_7 , C_{18} and C_{19} are land-use specific parameters that can be decided according to the vegetation cover variation in one year. These three parameters are estimated by non-linear regression under equation (7) for specific land use depending on a Landsat TM-derived NDVI (normalized vegetation cover index) data set (Su *et al.*, 2001, 2002).

Denitrification

Denitrification only occurs in oxygen-poor situations, associated with high water content (Krysanova *et al.*, 1998; Whitehead *et al.*, 1998a). In DNS, the user can

specify the threshold soil moisture content for denitrification:

$$\text{Denitrification} = k_3 C_8 [\text{NO}_3^-] \quad (8)$$

where C_8 is either 0 or 1 depending whether the soil moisture threshold is exceeded (i.e. 1 under moist soil conditions and 0 under dry conditions).

Mineralization

The flux of ammonium-N from organic matter mineralization is estimated using:

$$\text{Mineralization} = k_6 C_9 [\text{NH}_4^+] \quad (9)$$

where C_9 is associated with soil moisture conditions (i.e. 1 under moist soil moisture conditions and 0 at dry conditions). In DNS, it is assumed that the mineralization process is not limited by organic matter availability in each grid cell.

Atmospheric wet deposition

Wet deposition is the transfer of the nitrogen components from the atmosphere to the surface of the Earth within or on the surface of a hydrometeor (snow, hail or rainfall). In DNS, wet deposition from rainfall is estimated as:

$$\text{WetDeposition}_{[\text{NO}_3]} = C_{10} C_{12} \quad (10a)$$

$$\text{WetDeposition}_{[\text{NH}_4^+]} = C_{11} C_{12} \quad (10b)$$

where C_{12} is either 1 or 0 associated with whether runoff is generated or not.

Agricultural fertilizer input

A major problem in nitrogen modelling is how to distribute fertilizer inputs over time. In DNS, it is assumed that the fertilizer input (C_{13} or C_{14}) is available evenly over the first half of the growing season, then is available in a linearly decaying pattern for the remainder of the growing season. The fertilizer input to each grid cell of agricultural land is re-calculated depending on the fertilizer addition period (C_{15}) and start *DOY* of fertilizer addition (C_{16}).

Most of the fertilizer inputs are taken up by plants and the residues will enter the soil system. During rainy periods, the latter part will be washed away by surface runoff or leach into groundwater by infiltration. It is assumed that 30% of nitrate-N and 10% ammonium-N of fertilizer inputs are washed away from agricultural areas to stream-water by both surface and sub-surface runoff during rainy periods (Kunimatsu *et al.*, 1989).

Domestic discharge of nitrate- and ammonium-N

Due to no centralized wastewater treatment system in the study area, it is assumed that the domestic nitrogen is discharged in a diffusive way and evenly onto residential areas. The daily domestic nitrogen discharges ($\text{g N cell}^{-1} \text{ day}^{-1}$) are estimated as:

$$\text{DomesticNO}_3^- = C_{21}C_{23}AoP \quad (11a)$$

$$\text{DomesticNH}_4^+ = C_{22}C_{23}AoP \quad (11b)$$

Furthermore, it is assumed arbitrarily that only 10% of domestic discharges can contribute to stream water. *AoP* is the area of a grid cell in ha.

SIMULATION RESULTS AND SENSITIVITY ANALYSIS

Simulation results

Hydrological calibration of DXAJ is fulfilled by trial and error to obtain a better Nash coefficient (= 0.54); the hydrograph is shown in Fig. 3. Calibration of nitrogen modelling is difficult, not only because of the sparse water quality data used, but also because of the complexity of nitrogen processes inside the catchment. The third factor making nitrogen calibration difficult is that the nitrogen modelling is coupled with the hydrological component, which can not be modelled accurately. The inaccuracy of the hydrological modelling will affect the nitrogen modelling results.

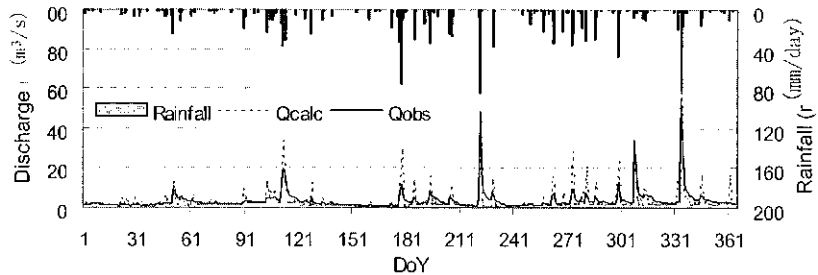


Fig. 3 Hydrological simulation in 1990 (Nash coefficient = 0.54).

The nitrogen calibrations focus on kinetic rate constants k_i ($i = 1 \dots 6$). The criteria for nitrogen calibrations are observed nitrate-N data at the water quality gauging station of the Mae sub-catchment. The calibrated kinetic rate constants are also shown in Table 2.

Depending on the calibrated parameters, the nitrogen dynamics at the Mae sub-catchment in 1990 are modelled (Fig. 4). Figure 4 includes the simulated nitrate /ammonium-N concentration, soil moisture deficit (SMD), air temperature, soil temperature and evapotranspiration.

The variation of SMD is closely related to rainfall pattern, both depth and temporal distribution, and evapotranspiration. For example, the SMDs in 1990 are high in May and June due to less rainfall and relatively high evapotranspiration in the corresponding periods. During the winter period, the SMDs are usually low due to very low evapotranspiration in the winter.

The estimation of soil temperature completely depends on the variation of air temperature and has a similar variation pattern with air temperature. The estimated evapotranspiration follows a similar variation pattern to air temperature.

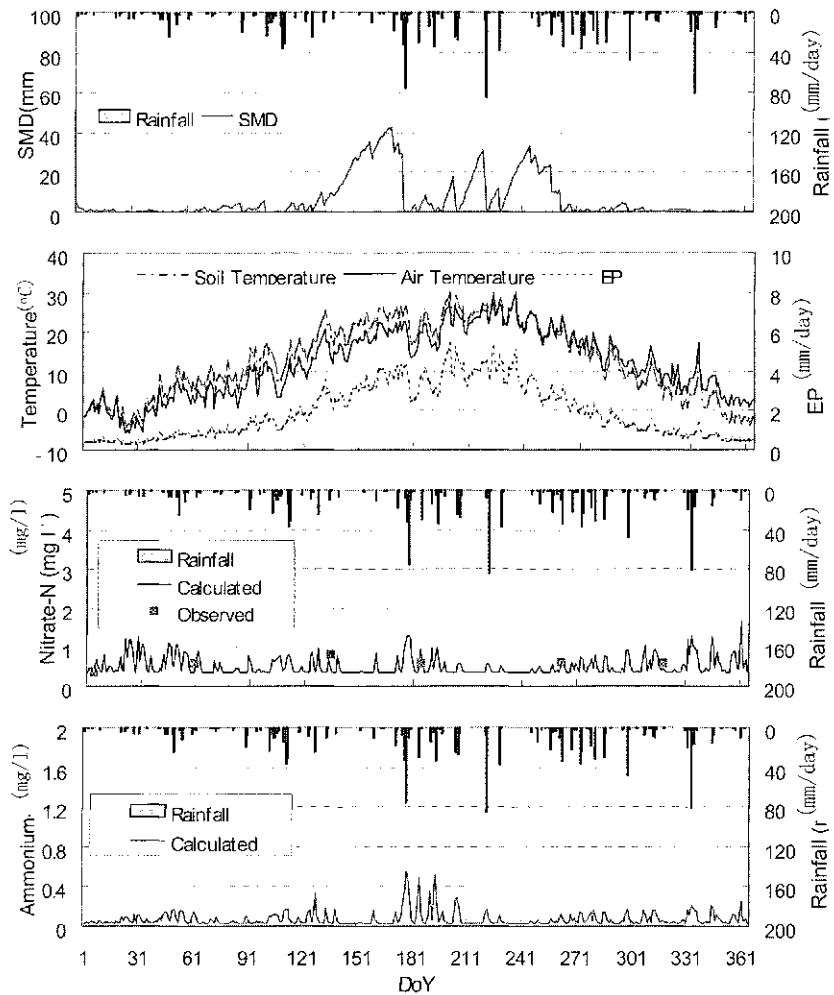


Fig. 4 Simulation results of nitrogen dynamics (1990).

The simulated nitrate-N concentration in Fig. 4 seems reasonable, because the sparse observed data points could fit the simulated ones well. However, it is too early to conclude whether it is good or not due to the sparse observed data used. Furthermore, most of water samplings were done in no-rain periods and the corresponding observed water quality data therefore only represents no-rain conditions. In the rainy periods and especially storm periods, there were no observed data to verify these simulated results. For the ammonium-nitrogen concentration, there was also no observed data to verify this result.

Sensitivity analysis

One-at-a-time sensitivity analysis is one of the simplest ways of investigating the sensitivity of a model (Hamby, 1994; Dubus *et al.*, 2000; Rankinen *et al.*, 2002). The

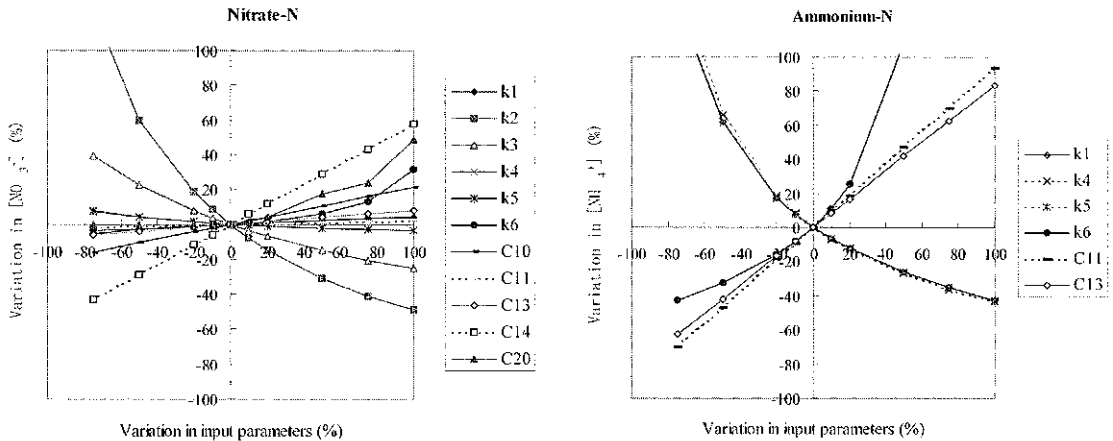


Fig. 5 Influence of variation of input parameters on nitrogen concentration modelled by DNS.

general framework is to repeatedly vary one parameter at a time while holding the others fixed. The model output when all parameters are kept constant at their nominal values is defined as the “base case”, and the sensitivity of the model is assessed by comparing the influence of the change of a given parameter with the base-case scenario.

Sensitivity analysis is conducted for parameters k_i ($i = 1, \dots, 6$), C_{10} , C_{11} , C_{13} , C_{14} and C_{20} . The base-case scenario is run using parameters in Table 2. The rainfall, evapotranspiration and meteorological data of year 1990 are used as known inputs to the DNS model in this sensitivity analysis.

The results of the influence of input parameters on the prediction of nitrate-/ammonium-N concentrations are presented graphically in Fig. 5. Values on the two axes are percentages, which means that direct comparison of the influence of the different parameters can be made. The closer the curve to the y-axis, the more influence a particular parameter has.

Depending on Fig. 5, the sensitivity level of focused parameters to nitrate-N concentration can be ranked as: $k_2 > C_{14} > k_3 > C_{20} > k_6 > C_{10} > (k_1/k_4/k_5/C_{11}/C_{13})$. The parameters in the parenthesis are at similar sensitivity level. It shows that plant uptake, k_2 , is the key sink of nitrate-N in the catchment, and the fertilizer application rate of nitrate-N, C_{14} , is the key source of nitrate-N in streamwater in the catchment.

Similarly, the sensitivity level of focused model parameters to ammonium-N concentration can be ranked as: $k_6 > (k_1/k_4/k_5) > C_{11} > C_{13}$. It shows that the ammonium mineralization process is the key source of ammonium-N, and nitrification, ammonium plant uptake and immobilization are the key sinks of ammonium-N in the catchment. Parameters k_2 , k_3 , C_{10} , C_{14} and C_{20} have no influence on the ammonium-N prediction.

CONCLUSIONS

The nitrogen dynamics modelling in this study is a good attempt at combining hydrological simulation and nitrogen processes at the catchment level. However, the

model calibration is difficult because of not only the sparse observed water quality data but also the complicated nitrogen processes in the soil–plant system. The information obtained in sensitivity analyses can be used to identify those parameters whose values require the most resources for their determination. This is useful in post-calibration and further studies. Furthermore, the following conclusions were made:

- Plant uptake is the key sink of nitrate-N, whereas agricultural fertilizer addition is the key source of nitrate-N. Wet deposition makes a relatively small contribution to the stream nitrate-N concentration.
- The denitrification process is ranked as the second most important sink of nitrate-N, because the study area is located in a humid area and the soil moisture content is always high, and so the denitrification process is very active in the catchment.
- Nitrification, plant uptake, and immobilization are the key sinks of ammonium-N, whereas ammonium mineralization is the key source of ammonium-N concentration.

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