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A semi-distributed Integrated Nitrogen model for multiple source assessment in Catchments (INCA): Part I — model structure and process equations

P.G. Whitehead[a,*], E.J. Wilson[b], D. Butterfield[a]

[a]Aquatic Environments Research Centre, Department of Geography, University of Reading, Reading, RG6 6AB, UK
[b]National Power Windmill Business Park, Swindon, UK

Abstract

A new model has been developed for assessing multiple sources of nitrogen in catchments. The model (INCA) is process based and uses reaction kinetic equations to simulate the principal mechanisms operating. The model allows for plant uptake, surface and sub-surface pathways and can simulate up to six land uses simultaneously. The model can be applied to catchment as a semi-distributed simulation and has an inbuilt multi-reach structure for river systems. Sources of nitrogen can be from atmospheric deposition, from the terrestrial environment (e.g. agriculture, leakage from forest systems etc.), from urban areas or from direct discharges via sewage or intensive farm units. The model is a daily simulation model and can provide information in the form of time series at key sites, or as profiles down river systems or as statistical distributions. The process model is described and in a companion paper the model is applied to the River Tywi catchment in South Wales and the Great Ouse in Bedfordshire. © 1998 Elsevier Science B.V.

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1. Introduction

Nitrogen inputs to the environment in fertiliser and sewage have been of interest for many years, largely driven by concerns for public water supplies and eutrophication in lowland rivers and lakes (Johnes, 1996; Whitehead, 1990). More recently, the role of atmospheric N inputs in both acidification and eutrophication of upland ecosystems and waters has been recognised (Skeffington and Wilson, 1988; Edwards et al., 1990; Woodin and Farmer, 1993; DOE, 1994; Langan and

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[*] Corresponding author.

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Wilson, 1997). Many forests in Europe are now viewed as 'N saturated' (Emmett et al., 1995), leaching N in excess of plant and microbial demand (Wilson and Emmett, 1997). This potentially has implications for water quality in downstream rivers and lakes, although a relationship between forest saturation and elevated river nitrate concentrations remains to be established.

The greatest threat to potable water quality arises from fertiliser application in areas of intensive agriculture (Whitehead, 1990), where N inputs can be 4–40 times higher than deposition from all atmospheric sources combined. Although much of the fertiliser is applied as ammonium and urea, N in excess of crop requirements can be nitrified and leached to groundwater as NO_3-N. Atmospheric N deposition generally makes a very small contribution to river nitrate concentrations in these agricultural catchments. In some lowland areas it may be becoming more significant however, due to increases in ammonia and NO_2 emissions coupled with lower agricultural inputs as a result of set aside and nitrogen sensitive area policies. As catchments become less dominated by agriculture or urban point sources, the atmospheric contribution becomes more important until, at the other end of the spectrum, atmospheric inputs in upland catchments can be a significant source of N. In these areas, the environmental impacts of nitrate leaching are primarily soil and surface water acidification rather than poor drinking water quality.

Nitrate levels in our rivers reflect the integration of a number of sources within the catchment including fertiliser inputs, atmospheric deposition and sewage discharges. Superimposed on these are 'natural' contributions from the mineralisation and nitrification of organic N in soils. In turn, these transformations will be influenced by climatic and seasonal factors (e.g. drought, temperature), and a number of land use and management practices such as afforestation, clear-felling, liming, ploughing and grazing. A river's nitrate profile will thus be a unique function of regional climate and catchment characteristics such as land use, urbanisation, short- and long-range deposition from emission sources, topography and hydrology. This integrated approach to chemical transport in catchments has been the focus of research in the LOIS project (Land Ocean Interaction Study, Wilkinson et al., 1997; Leeks and Jarvie, 1998). Neal et al. (1997, 1998) highlight the need to understand hydrochemical process interactions in order to predict fluxes of pollutants moving through catchments.

Due to the capacity of the catchment to store nitrogen — in soil, vegetation and ground water — it may take some time for the impacts of anthropogenic activity to be reflected in river nitrate quality. Similarly, the benefits of many of our environmental tools such as 'critical loads' and 'Nitrate Sensitive Areas' can only be assessed over long time scales. Because of this, models are essential for us to predict how changes in deposition, land use, management and climate will affect N loading to rivers. There has been a considerable amount of activity in the field of nitrogen modelling in the last few years. Many of the recently developed N models, such as MAGIC-WAND (Cosby et al., 1985a,b; Jenkins et al., 1997), MERLIN (Cosby et al., 1997), PNET-CN (Postek et al., 1995) and others (e.g. Thornley and Cannell, 1992) are directed towards upland ecosystems, forests or particular processes. Other process-based models have been developed for lowland agricultural systems to assess the impacts of fertiliser application on soils, ground- and surface waters (e.g. Addiscott and Whitmore, 1987; Cooper et al., 1993). These tend to be dynamic models which can provide short-term (weekly) information. Some models such as QUASAR (Whitehead et al., 1997; Whitehead and Williams, 1984) specifically address N dynamics in rivers, accounting for in-stream processes such as nitrification and denitrification. Despite all these developments, there are still very few models which integrate catchment and river processes. A recent model by Lunn (1995) addresses the whole catchment in a distributed manner but is driven by a complex hydrological model, SHE (System Hydrologic European; Abbott et al., 1986): alternative and companion approaches are also described in this special volume by Eatherall et al. (1998a,b), Cooper and Naden (1998) and Kowe et al. (1998). The export coefficient method of Johnes (1996) is a more pragmatic approach which models N dynamics empirically, based on observations and historical records of land use. This technique has proved very successful for estimating annual and seasonal nitrogen loads. However, the model is not process-based and cannot be used to generate daily variations in river N concentrations.

There is clearly a need for catchment N models which are both vertically integrated, tracking N inputs from the atmosphere and fertiliser through catchment soils to the river, and horizontally integrated, addressing the spatial variation across the catchment (e.g. land use, vegetation, hydrology) which influences nitrate levels down the river profile. INCA — an Integrated Nitrogen Catchment model — has been developed to bring all these elements together in a single model. It is:

- Dynamic — so that nitrogen concentrations and fluxes are produced as a daily time series, incorporating temporal variation in hydrological flow paths and N transformations in both catchment and river;
- Stochastic — so that parameter sensitivity can be assessed and outputs derived in probabilistic or percentile terms;
- Semi-distributed — so that the spatial variations in land use and management, effluent discharges and N deposition can be taken into account. (The term semi-distributed is used here, as it is not intended to model catchment land surface in a detailed manner. Rather, different land use classes and sub-catchment boundaries are modelled simultaneously and information fed sequentially into a multi-reach river model.)

INCA provides a tool to assess the contribution of N inputs from combustion, agriculture, urban and natural sources to catchment N pools and river nitrate concentrations. It can be used to address environmental and rural policy issues such as the impacts of land use change (e.g. increase or decrease in set-aside, crop switching), changes in the magnitude or distribution of NH_x and NO_x emissions, urbanisation, climate change and resource management practices. INCA will also enable us to investigate the link between forest saturation and exceedence of the critical N load for waters, as well as quantify the benefits of changing emissions on critical load exceedence.

2. The INCA model

The INCA model has been designed to investigate the fate and distribution of nitrogen in the aquatic and terrestrial environment. The model simulates flow pathways and tracks fluxes of both nitrate-N and ammonium-N in the land phase and riverine phase. The dynamic nature of the model means that the day-to-day variations in flow, N fluxes and concentrations can be investigated following a change in N inputs such as atmospheric deposition, sewage discharges or fertiliser application.

INCA has been designed to be easy to use, is fast, and has excellent output graphics. The menu system allows the user to specify the semi-distributed nature of a river basin or catchment, to alter reach lengths, rate coefficients, velocity-flow relationships, land use, temperature, rainfall and nitrogen deposition.

INCA provides the following outputs:

- Daily and annual land use-specific N fluxes for all transformations/processes within the land phase;
- Daily time series of flows, nitrate-N and ammonium-N concentrations at selected sites along the river;
- Profiles of flow and nitrogen concentrations along the river at selected times;
- Cumulative frequency distributions of flow and nitrogen at selected sites;
- Tables of statistics for all sites.

The model runs on any IBM compatible PC with MSDOS. Full details of the system requirements and installation are given in Butterfield and Whitehead (1997).

There are five components to modelling nitrogen in catchments using INCA.

1. A GIS interface which defines subcatchment boundaries and calculates the area of six land use classes in each subcatchment.

2. The Nitrogen Input Model which calculates the total N inputs from all sources to each sub-catchment, scaling dry deposition and fertiliser application according to land use.
3. The Hydrological Model which models the flow of effective rainfall in the reactive and groundwater zones of the catchment and within the river itself. This component of the model drives N fluxes through the catchment.
4. The Catchment Nitrogen Process Model which simulates N transformations in the soil and groundwater of the catchment. This component of the model includes plant uptake and microbial processes such as mineralisation, nitrification, denitrification etc.
5. The River Nitrogen Process Model which simulates dilution and in-river N transformations and losses such as nitrification and denitrification. Net N output from each sub-catchment (component model 4) provides the N flux into the corresponding river reach and input to the River Nitrogen Process Model.

Each of these components is considered in detail below.

2.1. The GIS interface for land use and sub catchment boundaries

INCA uses land use data to calculate N inputs to each sub-catchment from both dry deposition and fertiliser application, and modify certain N transformations in the land phase. The 18 land use classes within the ITE Land Cover Map of Great Britain (DoE Countryside Information System) have been aggregated into six classes for running INCA to simplify the interface with the N Input and Catchment N Process models (see Sections 2.2 and 2.4). The six land uses are forest, short vegetation (ungrazed), short vegetation (grazed, not fertilised), short vegetation (fertilised), arable and urban. The breakdown of ITE cover types within each of the six classes is given in Table 1.

These six land classes have to be mapped or superimposed onto a river basin and the percentage land use calculated for each sub-catchment. The sub-catchment boundaries are obtained from standard hydrological analysis based on topographic maps or automatically using a digital terrain model (DTM) and algorithms available in GIS systems such as ARC-INFO. We use algorithms developed by the Institute of Hydrology to determine principal sub-catchments which are then overlaid onto a 1-km map of the six INCA land classes on the GIS. The area of each sub-catchment and the percentage of each land class within it is calculated using the GIS. Part 2 of this paper gives a detailed description of this procedure as applied to the River Tywi Catchment in Wales.

Table 1
ITE land use cover types within INCA land classes

INCA land use class	ITE land cover map class
(1) Forest	Coniferous woodland (4) Deciduous woodland (5)
(2) Short vegetation (ungrazed)	Bog (1) Dense shrub/heath moor (6) Rough/marsh grass (12) Saltmarsh (13)
(3) Short vegetation (grazed, not fertilised)	Bracken (2) Heath/moor grass (7) Open shrub heath/moor (11)
(4) Short vegetation (fertilised)	Managed grassland (10)
(5) Arable	Tilled land (16)
(6) Urban	Inland bare (8) Suburban (15) Unclassified (17) Continuous urban (18)

2.2. The Nitrogen Input Model

Oxidised N inputs are estimated using MATADORN (Model of Atmospheric Transport and Deposition of Reacting Nitrogen, National Power 1997), a long-range transport and deposition model which treats emissions from low, high and continental/background sources, although other long-range transport models such as HARM or TRACE could also be used (Review Group on Acid Rain Report, 1997). Reduced N inputs are estimated using the Harwell Trajectory Model (HTM) (Review Group on Acid Rain Report, 1997). MATADORN calculates annual wet deposition of NO_2, HNO_3 and particulate nitrate on a 20-km cell scale using annual average concentrations and average rainfall. Total reduced N wet deposition (not disaggregated by source) on a 20-km scale is calculated in the same way by HTM. The dry deposition flux for NH_3 and each of the forms of oxidised N has been scaled according to the land use/vegetation type in the catchment using current best estimates of dry deposition velocity coefficients (v_g) (Fowler, personal communication). Values are available for forest, moorland and arable (Table 2). v_g for forest is used to calculate dry deposition to INCA land class 1, v_g for moorland is used for classes 2 and 3, and v_g for arable for INCA land classes 4 and 5.

The GIS-INCA interface outputs annual dry and wet total oxidised N, calculated from high, low and continental sources and dry and wet total reduced N deposition for each sub-catchment and each land use. Daily N loads (wet deposition) are calculated by multiplying the mean annual N concentration by daily rainfall. Rainfall data on a catchment scale are obtained from the United Kingdom Meteorological Office. Daily dry deposition is calculated as annual dry deposition/365. The final input file for deposition from the GIS-INCA interface is wet and dry reduced N deposition and wet and dry oxidised N deposition to each sub-catchment and land use. Separation of N sources and forms (reduced and oxidised) within the GIS-INCA interface gives the capability to compare the impacts of changing N emissions from different sources such as transport, power generation and agriculture.

Fertiliser inputs of N are calculated within INCA since they depend on the distribution of land use within the sub-catchment. Fertiliser application rates for different crops have been obtained from the Fertiliser Manufacturers Association. A major problem in nitrogen modelling is how to distribute fertiliser inputs over time (Addiscott and Whitmore, 1987). Within INCA it is assumed that the fertiliser is available evenly over the first half of the growing season then is available in an exponentially decaying pattern for the remaining half of the growing season.

2.3. The Hydrological Model

The Hydrological Model consists of three parts. Firstly, the MORECS soil moisture and evaporation accounting model (Meteorological Office, 1981) is used to convert daily rainfall data into an 'effective' rainfall time series. By effective we mean the water that penetrates the soil surface after allowing for interception and evapotranspiration losses. This hydrologically effective rainfall (HER) is used to drive the water transfers and nitrogen fluxes through the catchment system. The advantage of the MORECS model is that a daily time series of soil moisture deficit (SMD) is determined at the same time as HER, providing essential information for modelling soil moisture-dependent N transformations.

The second component of the hydrological model simulates the effect of land surface or topography on flow. A number of approaches can be used to model catchment flow pathways, ranging from time series techniques (Whitehead et al., 1979) through lumped hydrological models

Table 2
Dry deposition velocity coefficients to different vegetation types/land uses for each N form (personal communication Prof. D. Fowler, ITE)

	Dry deposition velocity (v_g) mm s^{-1}		
	Forest (INCA class 1)	Arable (INCA classes 4, 5)	Moor (INCA classes 2, 3)
NO_2	5	3	2
HNO_3	40	20	20
HNO_2	14	10	10
NO_3	6	[illegible]	1
NH_3	20	5	15

(Christophersen et al., 1982) to fully distributed models such as SHE (Abbott et al., 1986). In developing INCA, a semi-distributed approach has been adopted so that the dynamics of each sub-drainage basin can be characterised and incorporated into the overall system model. Hydrology within the catchment is modelled using a simple two box approach, with key reservoirs of water in the reactive soil zone and deeper groundwater zone (Fig. 1). It is necessary to know the principal residence time of these zones as well as the flow rates through soil and groundwater. The products of the complex nitrogen transformations in the soil reactive zone can enter the river system by two routes; lateral flow through the soil surface layers or vertical movement and transport through the groundwater zone. The flow model for these two zones can be written as

$$\text{Soil zone} \qquad \frac{dx_1}{dt} = \frac{1}{T_1}(U_1 - x_1) \qquad (1)$$

$$\text{Groundwater} \qquad \frac{dx_2}{dt} = \frac{1}{T_1}(U_8 x_1 - x_2) \qquad (2)$$

where x_1 and x_2 are output flows m^3 s^{-1} for the two zones and U_1 is the input driving hydrologically effective rainfall. T_1 and T_2 are time constants (i.e. residence times) associated with the zones and U_8 is the baseflow index (i.e. proportion of water being transferred to the lower groundwater zone). The baseflow index information can be obtained from the hydrological yearbooks (Institute of Hydrology, 1991) or from the application of time series modelling technique such as IHACRES (Jakeman et al., 1990). IHACRES uses a recursive approach to time series analysis to determine the dynamics of the two separate hydrological zones. It can be calibrated against rainfall and runoff data for sub-catchments to compute the baseflow separation, the soil zone time constant and the groundwater time constant.

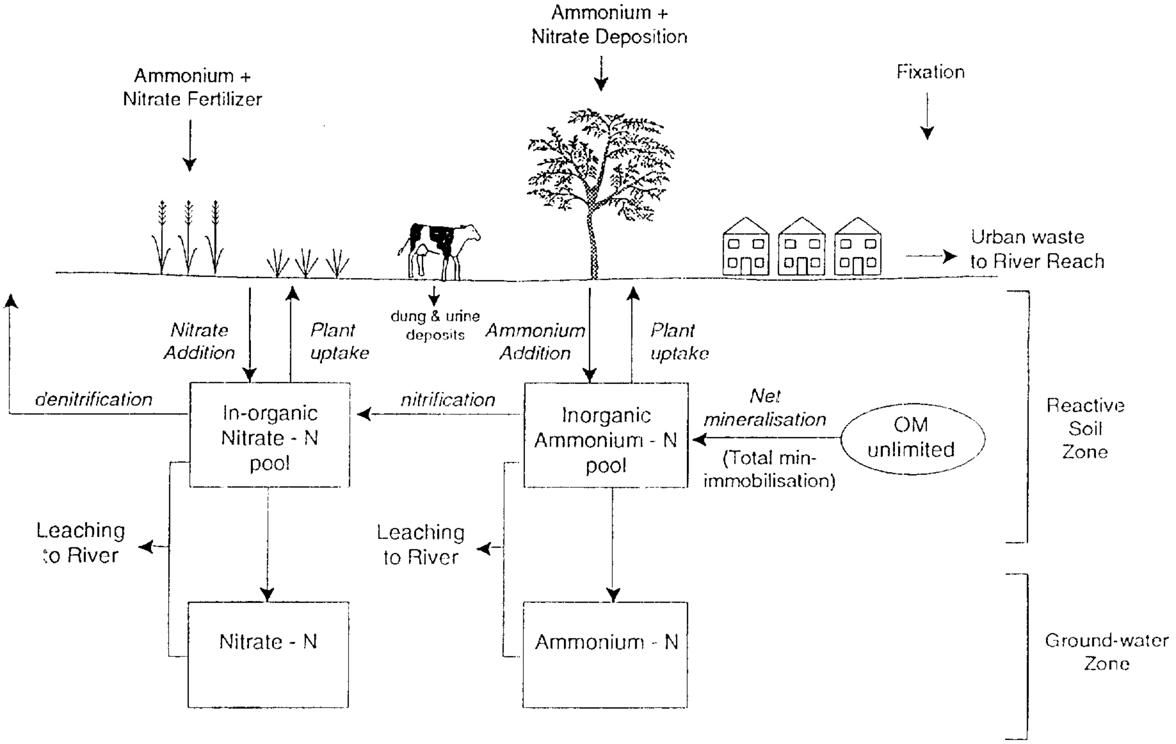

Fig. 1. Nitrogen inputs, processes and outputs in the soil and groundwater system.

The third component of the hydrological model is the river flow model. This model is based on mass balance of flow and uses a multi-reach description of the river system (Whitehead et al., 1979, 1981, 1997). Within each reach, flow variation is determined by a non-linear reservoir model. In hydrological flow routing terms the relationship between inflow, I, outflow, Q and storage, S, in each reach is represented by

$$\frac{\mathrm{d}S(t)}{\mathrm{d}t} = I(t) - Q(t) \tag{3}$$

where $S(t) = T(t) * Q(t)$, T is a travel time parameter, which can be expressed as

$$T(t) = \frac{L}{v(T)} \tag{4}$$

L is the reach length and v, the mean flow velocity in the reach (m s^{-1}). v is related to discharge, Q, through

$$v(t) = aQ(t)^b \tag{5}$$

where a and b are constants to be estimated from tracer experiments or from theoretical considerations. Whitehead et al. (1986) review alternative methods of estimating velocity-flow relationships in rivers. They conclude that an empirical approach using tracer experiments is preferable to theoretical estimation techniques. This is because tracer experiments integrate the actual behaviour of a river channel, whereas theoretical approaches are often limited by a need for physical channel information (which is often not available) and a detailed knowledge of channel roughness. A series of tracer experiments undertaken by the United Kingdom Environment Agency has generated velocity to flow information for many UK rivers. The Environment Agency has incorporated this information into the computer package IDRISI.

2.4. The Catchment Nitrogen Process Model

The Hydrological Model provides information on flow through the soil zone, the groundwater zone and the river system. Simultaneously whilst solving the flow equations it is necessary to solve the mass balance differential equations for nitrate-N and ammonium-N in both the soil and groundwater zones. The key processes and N transformations that occur in the land phase are shown in Fig. 1. INCA models plant uptake of ammonium-N and nitrate-N, nitrification, denitrification, mineralisation and immobilisation within each sub-catchment. INCA's Catchment Nitrogen Process Model uses a generalised set of equations with parameter sets specifically derived for the six different land classes. By modifying these parameters N fluxes from each of the transformations for a given land use can be calibrated against experimental and field data available in the literature. Certain processes such as plant uptake will vary according to land use in terms of both the rate of uptake and the seasonal pattern of uptake. For example, spring-sown arable crops will have a shorter growing season than coniferous forests but a higher rate of N utilisation. Microbial N transformations within the soil are temperature and moisture dependent, both of which can vary according to land use. Soil temperatures will be modified by the vegetation cover; in summer, soil temperatures in fields will be higher than in deeply shaded coniferous forests, for example. The second factor, soil moisture, will also vary through the catchment. Upland areas with podsolic and peaty soils will have greater water retention compared with better draining soils in lowland agricultural areas. Within INCA, land use can be viewed as an approximate surrogate for soil type for a number of characteristics which influence N transformations, although the effect of more complex soil properties such as % C and N, and C:N ratio are not accounted for in the model.

The Catchment Nitrogen Process Model takes the output from the Nitrogen Input Model (INCA-GIS interface), which gives wet and dry ammonium-N and nitrate-N inputs from atmospheric deposition, together with N fixation and fertiliser input to each land use sub-catchment. An initial condition is also required for surface and groundwater concentrations. In a sense, the initial conditions represent the history of the catchment and land use at that point in time. The user therefore needs to either measure groundwater and soil water nitrogen as input initial condition or estimate these from model calibration against field data.

As shown in Fig. 1 the soil reactive zone leaches water to the deeper groundwater zone and the river. In the groundwater zone it is assumed that no biochemical reactions occur and that a mass balance of NH_4-N and NO_3-N is adequate. The equations used in INCA are as follows.

2.4.1. Nitrate-N

Soil zone
$$\frac{dx_3}{dt} = \frac{1}{V_1}(U_3 - x_1x_3) - \underbrace{C_3U_7x_3}_{\text{plant uptake}} + \underbrace{C_6x_5}_{\text{nitrification}} - \underbrace{C_1U_5x_3}_{\text{denitrification}} + \underbrace{C_2}_{\text{fixation}} \qquad (6)$$

Groundwater zone
$$\frac{dx_4}{dt} = \frac{1}{V_2}(x_3x_1U_8 - x_2x_4) \qquad (7)$$

2.4.2. Ammonium-N

Soil zone
$$\frac{dx_5}{dt} = \frac{1}{V_1}(U_4 - x_1x_5) - \underbrace{C_{10}U_7x_5}_{\text{plant uptake}} - \underbrace{C_6x_5}_{\text{nitrification}} + \underbrace{C_7U_6}_{\text{mineralisation}} - \underbrace{C_8x_5}_{\text{immobilisation}} \qquad (8)$$

Groundwater zone
$$\frac{dx_6}{dt} = \frac{1}{V_2}(x_5x_1U_8 - x_2x_6) \qquad (9)$$

where x_3 and x_4 are the daily NO_3-N concentrations, mg l^{-1}, in the soil zone and groundwater zone, respectively. x_5 and x_6 are the daily NH_4-N concentrations, mg l^{-1}, in the soil zone and groundwater zone, respectively. V_1 and V_2 are the equivalent water volumes for the soil and groundwater zones respectively and where

$$V_1 = T_1x_{1m} \text{ and } V_2 = T_2x_{2m}$$

where subscript m refers to the mean flow. U_8 is the baseflow index and C_3, C_6, C_1, C_2, C_{10}, C_7, C_8 are rate coefficients (days^{-1}) for plant uptake of nitrate, nitrification, denitrification, non-biological N fixation, plant uptake of ammonium, mineralisation, immobilisation. U_3 and U_4 are the daily nitrate-nitrogen and ammonium-nitrogen loads entering the soil zone and constitute the additional dry and wet deposition and agricultural inputs (e.g. fertiliser addition). All rate coefficients are temperature dependent using the equation

$$C_n = C1.047^{(\theta_s - 20)}$$

where θ_s is soil temperature estimated from a seasonal relationship dependent on air temperature as follows

$$\text{Soil temperature} = \text{air temperature} + C_{16}\,\sin\left(\frac{3}{2}\pi\frac{\text{day no.}}{365}\right)$$

where C_{16} is the maximum temperature, °C, difference between summer and winter conditions (Green and Harding, 1979).

This relationship generates a seasonal pattern for each land use, which is controlled by the parameter C_{16}. Daily catchment average air temperature is thus required as input data to the Catchment Nitrogen Process Model within INCA and these data are available from the UK Meteorological Office.

Whilst it is assumed that no process transformations except dispersion occur in the groundwater zone, there are major nitrogen transformations occurring in the soil reactive zone. Each process is represented in the above soil equations and each of these is now described.

2.4.3. Plant uptake

While there is some evidence that different ecosystems and even different species preferentially utilise either nitrate-N or ammonium-N, there are insufficient data to build this into the model. In INCA, plant uptake of ammonium-N and nitrate-N occurs in proportion to the availability of the two forms in the soil reactive zone, with a ceiling maximum uptake rate. The maximum uptake rates can be set by the user and may vary from crop to crop or with different tree species or age profiles. The general form of the uptake term used in Eqs. (6) and (8) is as follows:

$$\text{Uptake} = C_n U_7 x_n$$

where C_n is the uptake rate (days^{-1}) and x_n is the available nitrate-N or ammonium-N concentration. U_7 is a seasonal plant growth index (after Hall and Harding, 1993) where

$$U_7 = 0.66 + 0.34 \sin\left(2\pi \frac{[\text{day no.} - C_{11}]}{365}\right).$$

Within INCA the user can specify the growing season. C_{11} is the day number associated with the start of the growing season.

2.4.3.1. Mineralisation-immobilisation. The flux of ammonium from organic matter mineralisation is calculated from:

$$\text{Net mineralisation} = C_7 U_6 - C_8 x_5$$

where C_7 and C_8 are mineralisation and immobilisation rates (days^{-1}), respectively. x_5 is the ammonium-nitrogen concentration (mg l^{-1}). U_6 is a soil moisture driven term such that U_6 is 1 under moist soil moisture conditions and 0 at low soil moisture conditions, i.e.

$$U_6 = \frac{\text{SMD} - \text{SMD}_{\text{max}}}{\text{SMD}_{\text{max}}}$$

where SMD is the daily soil moisture deficit (mm). N return in litterfall is not specified in the model, but it is assumed that mineralisation is not limited by organic matter availability.

2.4.3.2. Nitrification. The flux of nitrate from nitrification is estimated as:

$$\text{Nitrification} = C_6 x_5$$

where C_6 is the nitrification rate (days^{-1}) and x_5 is the ammonium concentration (mg l^{-1}).

2.4.3.3. Denitrification. Denitrification only occurs under moist soil conditions. Within INCA, the user can specify the threshold soil moisture content for denitrification.

$$\text{Denitrification} = C_1 U_5 x_3$$

where C_1 is the denitrification rate (days^{-1}). U_5 is either 0 or 1 depending on whether the soil moisture threshold is exceeded (i.e. 1 under wet conditions and 0 under dry conditions).

2.4.3.4. Fixation. Non-biological fixation of atmospheric N_2 (e.g. by electrical discharge) is assumed to occur at a fixed rate, C_2 (mg l^{-1} day^{-1}). This rate C_2 is recalculated in the model in terms of kg N/ha/year.

Thus all the key processes controlling nitrogen behaviour are incorporated into the model equations. As shown in Fig. 1, N from the soil reactive zone and groundwater zone leaches into the river. N transformation and fluxes in the river are simulated by a set of river equations in the river N process model.

2.5. The River Nitrogen Process Model

The River Nitrogen Process Model treats ammonium-N and nitrate-N inputs from the Catchment Nitrogen Process Model (soil reactive zone and groundwater zone sources) and N inputs from the direct discharge of sewage effluent and urban runoff. The key processes operating in each reach of the river are nitrification and denitrification and are shown in Fig. 2. The reach mass balance must include the upstream nitrate-N and ammonium-N in addition to the catchment and effluent inputs.

The equations for the flow, nitrate-N flux and ammonium-N flux in the river reaches are then

$$\text{Flow} \qquad \frac{\mathrm{d}x_7}{\mathrm{d}t} = \frac{1}{T_3}(U_9 - x_7) \qquad (10)$$

$$\text{Nitrate} \qquad \frac{\mathrm{d}x_8}{\mathrm{d}t} = \frac{1}{V_3}(U_{10}U_9 - x_7 x_8) - C_{17} x_8 + C_{14} x_9 \qquad (11)$$

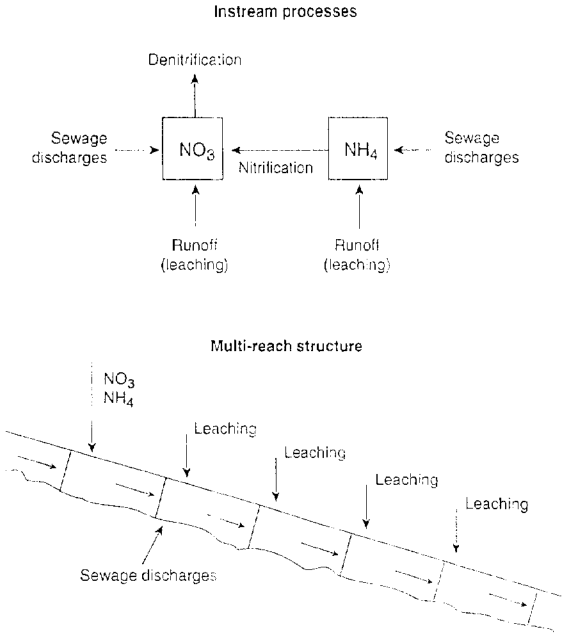

Fig. 2. Nitrogen inputs, processes and outputs in the river system.

$$\text{Ammonium}\quad \frac{dx_9}{dt} = \frac{1}{V_3}(U_{11}U_9 - x_7x_9) - C_{14}x_9 \qquad (12)$$

where

$$V_3 = T_3x_7$$

and

$$T_3 = \frac{L}{v} = \frac{L}{aQ^b}.$$

T_3 is the reach residence time and is derived from a non-linear velocity flow relationship as described previously. U_9 is the sum of upstream flows from the previous river reach, sub-catchment runoff and sewage discharge. U_{10} is the flow weighted upstream NO_3-N, mg l^{-1}, based on NO_3-N from the previous river reach, sub-catchment runoff and sewage works. U_{11} is the flow weighted upstream NH_4-N, mg l^{-1}, based on NH_4-N from the previous river reach, sub-catchment runoff and sewage works. x_7 is the estimated downstream flow rate, m^3 s^{-1}. x_8 and x_9 are the downstream (i.e. reach output) concentrations of nitrate and ammonia, respectively. C_{17} and C_{18} are temperature-dependent rate parameters for denitrification and nitrification, respectively. Temperature effects are introduced related to river water temperature, θ_w, as follows

$$C_n = C\ 1.047^{(\theta_w - 20)}.$$

Fig. 2 shows the processes operating in the river system and the multi-reach structure of the river model. Water flows from the sub-catchments to drain into the river reaches and the river equations are solved to maintain a mass balance along the river. Additional inputs from sewage effluents or industrial discharges can be incorporated into the reach structure mass balance and the user specifies these inputs.

The combined set of nine differential equations and related parameters are all solved simultaneously using a 4th order Runge Kutta integration routine, with a Merson variable step length to ensure accurate and fast numerical solution. Moreover, this procedure ensures stable numerical integration of the equations.

3. Discussion and conclusions

INCA attempts to model all the key processes governing the fate of N inputs to catchments, and this has required certain assumptions to be made. One of the most difficult aspects to model is fertiliser application. While the N input to the catchment is known, the availability of this N to plants and microbes will depend on the rate of dissolution of the solid fertiliser which in turn will be determined by the particular weather conditions following application. The residence time of fertilisers and factors controlling runoff have been key issues for agricultural scientists for many years (Addiscott and Whitmore, 1987). Other factors such as the starting N status of the soil which will influence the microbial sink for N and hence the fraction of N inputs that are leached, are also difficult to build into generalised catchment models. A further limitation of INCA is that the variation in N demand across forests of different ages or types is not accounted for, rather it models an 'average' stand. However, the user can tailor the process parameters to reflect the nature of the forests within the particular catchment they are modelling. Clearly, extensive calibration and validation exercises are required with process-based models such as INCA, to ensure that the assumptions made are robust.

Part 2 of this paper looks at model calibration and describes in detail the application of INCA to the upland River Tywi in South Wales and to the Great Ouse in the Bedfordshire lowlands. Two calibration methods are explored: one method compares annual mean fluxes with experimental and field data from around the world, while the other method compares model output with measured stream flow and chemistry. These two catchments have very different land use and hydrological regimes and indicate the wide applicability of INCA. In addition a parameter sensitivity analysis is undertaken. One of the major advantages of INCA is that it can potentially be applied to any catchment. The next step is to test INCA against a wider range of sites with different hydrology and chemical characteristics to build confidence in the use of the model for all types of catchment.

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