Extracting the Essence of Process-Based Models of the Flow of Nitrogen through Catchments

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Abstract
The dynamic properties of process-oriented models of the flow of nitrogen through catchments can be very complex. We introduced several types of ensemble runs that can provide informative summaries of meteorologically normalised model outputs and also clarify the extent to which such outputs are related to various model parameters. Specifically, we showed how to assess travel times for nitrogen and water in the unsaturated and saturated zones. Studies of the catchment model INCA-N revealed that the temporal distribution of the modelled water quality response to changes in fertiliser application was determined primarily by the hydromechanical parameters of the model, whereas the magnitude of the total intervention effect was influenced mainly by the parameters governing the turnover of nitrogen in soil. Furthermore, the travel times in this model were invariably shorter for nitrogen than for water due to preferential removal of the nitrogen exhibiting unusually long residence times.

1. Introduction
Numerous process-oriented deterministic models have been developed to explain and predict the flow of nitrogen through catchments (e.g., Arheimer & Brandt, 1998; Heng & Nikolaidis, 1998; Kroes & Roelsma, 1998; Whitehead *et al*., 1998a,b; Refsgaard *et al*., 1999). In general, such models can satisfactorily describe prevailing spatial distributions of riverine loads of nitrogen. Also, they can usually clarify most of the seasonal variation and a considerable fraction of the short-term temporal fluctuations in the nitrogen loads. However, it is less certain how well the models can predict several-year-long lags in the water quality response to interventions in a drainage area. In addition, the complexity of the cited models can make it difficult to comprehend the relationships between model parameters and the predicted impact of interventions.

The present study was devoted to model reductions that can help extract the essence of complex process-oriented models that are driven by meteorological data. Specifically, different types of ensemble runs were introduced in which natural fluctuations in the model output were suppressed by computing the average output for a collection of artificially generated time series of rainfall and temperature data. Some of these ensemble runs were designed to elucidate the fate and travel times of nitrogen applied on the soil surface. Another group of simulation experiments aimed to clarify water travel times in the unsaturated and saturated zones.

The above-mentioned techniques were used to determine how changes in fertiliser applications affect the riverine loads of inorganic nitrogen predicted by the Integrated Nitrogen in Catchments (INCA-N) model (Whitehead *et al*., 1998b). Time series of meteorologically normalised nitrogen loads were computed, and the results were summarised in impulse-response functions. We also examined which model parameters had the greatest influence on the total response and the time lag between intervention and response.

2. The INCA-N model

The INCA-N is a semi-distributed, process-based model of the flow of water and nitrogen through catchments (Wade *et al*., 2002). INCA-N simulates the key factors and processes that affect the amount of NO_3 and NH_4 stored in the soil and groundwater systems, and it feeds the output from these systems into a multi-reach river model. The final output of the INCA-N model consists of daily estimates of water discharge and NO_3 and NH_4 concentrations in stream water at discrete points along the main channel of the river.

INCA-N takes the following input fluxes into account: atmospheric deposition of ammonium and nitrate (wet and dry), application of NO_3 and NH_4 fertilisers, mineralisation of organic matter (yielding NH_4), nitrification (yielding NO_3), and nitrogen fixation. From these data, various output fluxes (plant uptake, immobilisation, and denitrification) are subtracted before the amount available for stream output is calculated.

Whenever relevant, inputs and outputs are differentiated by landscape type and varied according to environmental conditions (soil moisture and temperature). The model also simulates the flow of water from different kinds of land use through the plant/soil system in order to deliver the nitrogen load to the river system. The load is then routed downstream, after accounting for direct effluent discharges and in-stream nitrification and denitrification.

3. Study area

The empirical data we used were collected in the Tweed River Basin, which is located in Scotland (4300 km^2) and England (680 km^2). The land-phase data included information about land use in 23 sub-basins, whereas the meteorological inputs (air temperature and precipitation) were assumed to be the same for the entire Tweed Basin (Jarvie *et al*., 2002).

The catchment of the River Tweed consists of a horse-shoe-shaped rim of hills composed of older, harder rocks which surround a relatively flat basin of younger rocks covered with a thick layer of glacial debris. The land cover ranges from heather moorlands and rough grazing on the hills, improved pastures on the lower slopes to arable land in the lowlands, and the average application of inorganic nitrogen on cultivated land is 106 kg/ha/yr. Average rainfall is about 650 mm in the lower reaches of the catchment and considerably higher in the highlands. The base-flow index is estimated to approximately 0.5 for all sub-basins.

4. Simulation methods

4.1 Notation

From a mathematical point of view, the INCA-N model and other deterministic substance transport models can be regarded as functions

$$y = f(\boldsymbol{x})$$

The output is a scalar or a vector of moderately high dimension, whereas $\boldsymbol{x}$ can contain a very large number of components. We introduce the notation $\boldsymbol{x}(t, z)$ to show that at least some of the components of $\boldsymbol{x}$ can depend on time (t) and location (z). Moreover, we write

$$z_j \prec z_k$$

to indicate that z_j is located upstream of z_k and

$$\boldsymbol{y}(t, z_k) = f(\boldsymbol{x}(s, z_j), s \le t, z_j \prec z_k)$$

to indicate that the output at time t is a function of both current and previous inputs to all sub-basins upstream of the location under consideration. Different types of model inputs are separated by setting

$$\boldsymbol{x}(s,z) = (\boldsymbol{u}(t_0, z), \boldsymbol{v}(s,z), \boldsymbol{w}(s,z), \boldsymbol{\theta}(z))$$

where

$\boldsymbol{u}(t_0, z)$ defines the state of the system at time t_0;
$\boldsymbol{v}(s, z)$ is a vector representing the anthropogenic forcing of the system;
$\boldsymbol{w}(s, z)$ is a vector representing the meteorological forcing of the system; and
$\theta(z)$ is a vector of model parameters.

The vector $\boldsymbol{u}(t_0, z)$ contains information about water content and concentrations of various nitrogen species in different parts of the system at the onset of the observation period. Information about fertiliser use can exemplify the content of $\boldsymbol{v}(s, z)$, and $\boldsymbol{w}(s, z)$ can contain data on air temperature and precipitation. The vector $\theta(z)$ includes hydrogeological parameters and rate coefficients for nitrogen transformation processes. Unless otherwise stated, we regard riverine loads of inorganic nitrogen (NO_3-N + NH_4-N) as the primary response variable.

4.2 Meteorological normalisation

Meteorological normalisation aims to remove or suppress the impact that random variation in weather conditions has on the model output. We performed so-called conditional normalisation, i.e., the predicted riverine load of inorganic nitrogen was averaged over different meteorological forcings, while the anthropogenic inputs were fixed (Grimvall *et al*., 2001; Forsman & Grimvall, 2003).

A set $\{\boldsymbol{w}_i, i = 1, \dots, n\}$ of artificial meteorological inputs with approximately the same statistical properties as the original data series was created by resampling blocks of observed weather records. Specifically, 30-day-long blocks were sampled, each of which was randomly selected from the different observation years with a shift of up to 15 days in the Julian day. Thereafter, the model was run for each element of $\{\boldsymbol{w}_i, i = 1, \dots, n\}$, and the mean output

$$\bar{\boldsymbol{y}}(t, z_k) = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{f}((\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}_i, \boldsymbol{\theta}), s \le t, z_j \prec z_k)$$

was computed for each time point t. A total of 400 replicates of the meteorological forcing was found to be sufficient to remove the weather-dependent variation in the model output.

4.3 Ensemble runs elucidating the fate and travel time of nitrogen

Laboratory and field experiments involving labelled nitrogen species have contributed substantially to current knowledge regarding the turnover of nitrogen in soil (e.g., Shen *et al*., 1989). Any process-oriented model that can accommodate user-defined time series of fertiliser inputs can be employed to mimic important features of such experiments.

Let $\boldsymbol{v}(s, \cdot)$ designate a given fertilisation scheme and let $\Delta\boldsymbol{v}(s, \cdot)$ denote a minor change in that scheme. We can then compute the difference

$$\Delta\bar{\boldsymbol{f}} = \bar{\boldsymbol{f}}(\boldsymbol{u}, \boldsymbol{v} + \Delta\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\theta}) - \bar{\boldsymbol{f}}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\theta}) \qquad (1)$$

for each time point t. If $\Delta\boldsymbol{v}(s, \cdot) = 0$ for the second year and onwards, such calculations can provide information about the fate of the nitrogen applied during the first year. Moreover, we can compute impulse response functions for the impact of fertiliser application on riverine loads of nitrogen.

4.4 Ensemble runs elucidating the travel time of inert substances and water

If all processes involving transformation or immobilisation of nitrogen are switched off, the ensemble runs mentioned in the previous section can provide information about the travel time of an inert substance. In that case the flow of water is the only transport mechanism, thus such ensemble runs also reveal the travel times of water through the unsaturated and saturated zones. In particular, it can be established whether the nitrogen delivered from land to surface water is younger or older than the water reaching the stream.

5. Results

Ensemble runs were made for a variety of systems ranging from a soil column to entire catchments. The simplest systems were defined as catchments with a single sub-basin and a single land-use category. Furthermore, all in-stream processes, including abstraction of river water and direct emissions to the river, were switched off when a single land use category was in focus. The base-flow index was varied from zero to one in order to highlight the role of groundwater in the riverine loads of nitrogen.

5.1 Nitrogen retention in simple systems

The INCA-N model was first used to simulate the output of nitrogen from systems consisting of a single sub-basin comprising only arable land or only forest. The weather-dependent interannual variation in riverine loads of inorganic nitrogen was removed by computing averages over an ensemble of runs representing different meteorological inputs, and the meteorologically normalised response to impulses in the input (i.e., applications or deposition) of nitrogen was examined.

When the application of fertilisers or the atmospheric deposition of nitrogen was increased the first year of the study period, the values of $\Delta\bar{f}$ (Eq. 1) were positive for a sequence of years. Figure 1 illustrates two general features of the water quality response in systems with base-flow index zero. First, the time delay in the response was relatively small in such systems. Second, the cumulated increase in riverine loads was considerably smaller than the impulse in nitrogen input. In systems comprising arable land, removal of nitrogen through harvesting and denitrification attenuated the water quality response to changes in fertiliser application. In forest systems, long-term storage of nitrogen in the biomass (and denitrification) almost eliminated the response to changes in the wet and dry deposition of inorganic nitrogen.

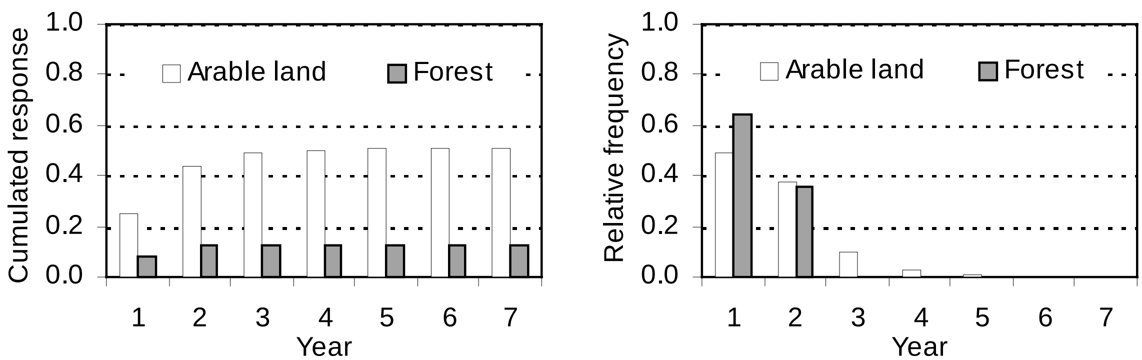

Figure 1. Predicted response of riverine loads of inorganic nitrogen to impulses in fertiliser inputs on arable land and atmospheric deposition on forests during the first year of the study period. The diagram to the left shows the ratio of the cumulated increase in riverine loads to the magnitude of the impulse, and the diagram to the right illustrates the relative frequency of travel times for the extra nitrogen supplied to the system. The base-flow index was zero in all simulations.

Figure 2 illustrates the dynamic properties of systems with base-flow index one. As expected, the time lag in the water quality response increased with the base-flow index due to the increased influence of groundwater. However, the total intervention effect was unchanged, because the INCA-N model does not include any transformation or immobilisation of nitrogen in the saturated zone.

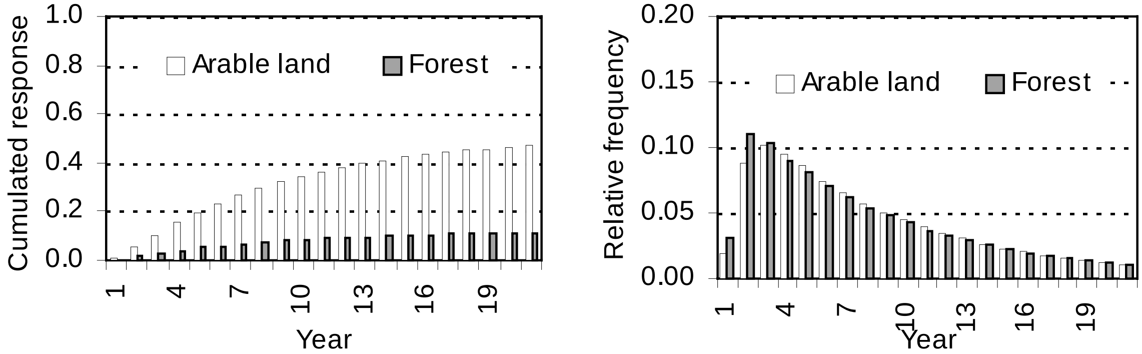

Figure 2. Predicted response of riverine loads of inorganic nitrogen to impulses in fertiliser inputs on arable land and atmospheric deposition on forests during the first year of the study period. The diagram to the left shows the ratio of the cumulated increase in riverine loads to the magnitude of the impulse, and the diagram to the right illustrates the relative frequency of travel times for the extra nitrogen supplied to the system. The base-flow index was set to one. All other conditions were the same as in Figure 1.

Because the INCA-N model is non-linear the response to an impulse in fertiliser application varies with the rate of application before and after the impulse. This is illustrated in Figure 3, which shows that strongly fertilised systems respond more clearly to changes in the nitrogen input. If we had also taken into account that different levels of fertiliser application are associated with different initial concentrations of nitrogen species in soil, the difference between the two ensemble runs would have been larger and would already have emerged the first year.

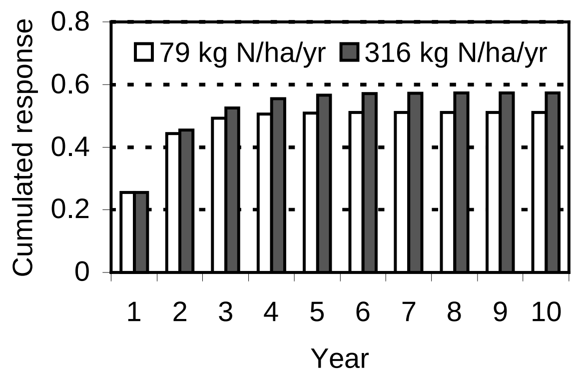

Figure 3. Ratio of the increase in riverine loads of nitrogen to the magnitude of the impulse in fertiliser application in two systems respectively receiving 79 and 316 kg N/ha/yr.

5.2 Water residence times in simple systems

Ensemble runs of the type defined in section 4.4 were undertaken to elucidate the water residence times in the unsaturated and saturated zones. The results obtained for simple systems comprising only arable land or only forests are illustrated in Figure 4. It is especially noticeable that, on average, the inorganic nitrogen reaching the river has a shorter travel time than the water in which it is dissolved. This is due to the fact that denitrification and plant uptake result in preferential removal (or uptake) of the nitrogen that has unusually long residence times.

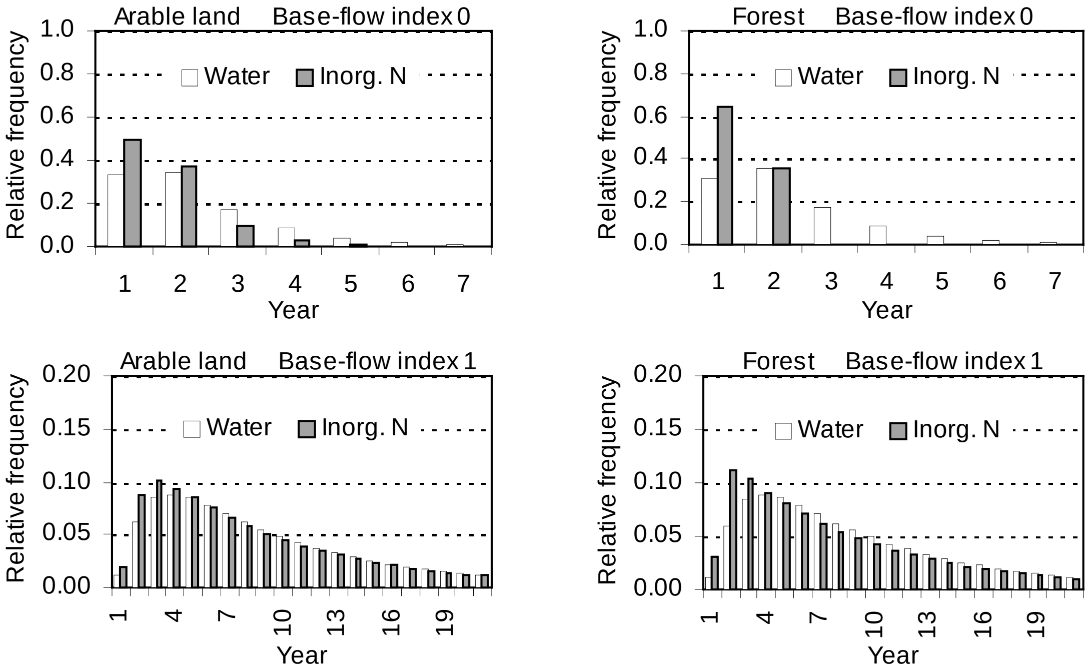

Figure 4. Predicted relative frequencies of travel times for inorganic nitrogen and water in the systems defined in Figures 1 and 2. The base-flow index was set to zero (top) or one (bottom).

5.3 Sensitivity analysis of the predicted response to changes in fertiliser application

The INCA-N model does not include any transformation or immobilisation of nitrogen in the saturated zone. Under such circumstances it is obvious that long residence times in groundwater will cause long time lags in the water quality response to land-use interventions in the drainage area. It is also clear that high rates of denitrification in soil and uptake by plants will reduce the total intervention effect. However, it is not as apparent how the parameters governing nitrogen turnover in soil influence the travel time for the nitrogen that is leached from land to surface water.

Figure 5 illustrates that, in the INCA-N model, the length of the delay in water quality response is practically independent of the mineralisation rate. Further information about the sensitivity of predicted intervention effects to selected model parameters is given in Table 1. The values given for total response in the table represent the percentage of the nitrogen applied on arable land that (eventually) reaches the river. The relative importance of (almost) direct response is expressed as p_1+p_2, where $\{p_i, i = 1, 2, \ldots\}$ is the probability distribution of the time lags for the nitrogen that reaches the river.

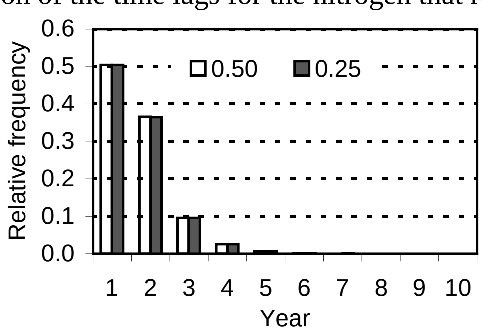

Figure 5. Predicted travel times of nitrogen in a system consisting of a single sub-basin comprising only arable land and with a base-flow index of zero. Mineralisation rates (kg N ha^{-1} yr^{-1}) are indicated in the graph.

5.4 Simulations of catchment-scale retention

When the INCA-N model is used to simulate the flow of water and nitrogen through a whole catchment, the total delivery of nitrogen to the river is computed by summing all inputs to the different parts of the river. The load of inorganic nitrogen at the mouth of the river can be considerably smaller due to in-stream processes (Behrendt & Opitz, 1999). In addition, point emissions, atmospheric deposition on water surfaces, and abstraction of water can have an impact on the riverine loads of nitrogen and the response to interventions in the drainage area.

There are no major lakes in the Tweed Basin, hence in-stream processes will have only a small effect on the total travel times of nitrogen and water through the catchment. Figure 6 illustrates that the in-stream processes also have only a very small impact on the cumulated response of riverine loads to an impulse in fertiliser application.

Table 1. Total effect of the intervention and relative importance of almost direct response to changes in fertiliser application in relation to the rates of different natural processes (N, nitrification; U, plant uptake; D, denitrification). The base-flow index was zero and the mineralisation rate was 0.5 (kg N ha^{-1} yr^{-1}).

Process rate			Total response (%)	Almost direct response ($p_1 + p_2$)
N (day^{-1})	U (day^{-1})	D (day^{-1})		
0.02	0.02	0.001	51	0.87
0.04	0.02	0.001	52	0.87
0.02	0.01	0.001	64	0.81
0.04	0.01	0.001	65	0.81
0.02	0.02	0.005	44	0.91
0.04	0.02	0.005	43	0.91
0.02	0.01	0.005	53	0.87
0.04	0.01	0.005	53	0.87

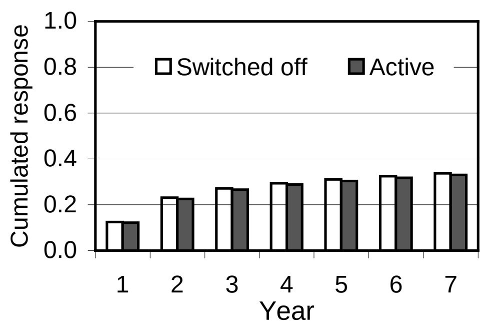

***Figure 6**. Predicted response in riverine loads of nitrogen to an impulse (1% increase) in fertiliser application in the entire Tweed Basin during the first year of the study period. In-stream processes and direct inputs to water were either switched off or active in the model simulations.*

6. Discussion

This study shows that ensemble runs involving artificially generated meteorological inputs can be employed to extract model features that might otherwise be hidden by the total variation in the model output. Introducing ensemble runs clarified how water and nitrogen travel times in the saturated and unsaturated zones contribute to time lags in the river response to interventions in the drainage area.

The simulation techniques described here facilitate comparative studies of different catchment models. Also, ensemble runs provide useful input to sensitivity analyses of model outputs. The results obtained with the INCA-N model indicate that the total intervention effect was influenced mainly by the parameters governing the turnover of nitrogen in soil, whereas the temporal distribution of the water quality response was determined primarily by the hydromechanical parameters of the model.

Moreover, we found that, almost regardless of the model parameters, there was a relatively rapid response to interventions in the drainage area. This seems to contradict the absence of an unambiguous water quality response in many Eastern European river basins, where agricultural practices changed dramatically in the early 1990s (Stålnacke *et al*., 2003).

Two potential explanations for our observations call for further discussion. The first of these is hydrogeological in nature and concerns the fact that the groundwater residence times are rather long in many river basins in the Baltic Republics and Poland, and the monitoring programmes may have failed to detect the water quality changes that have actually taken place. The second explanation is directly related to the INCA-N model. Analyses of ^{15}N-labelled fertiliser residues in the soil have clearly demonstrated that the dominating pathway of inorganic nitrogen in soil includes uptake by plants and subsequent mineralisation of plant residues (Shen *et al*., 1989), and these conditions can apparently prolong the travel time of nitrogen in the unsaturated zone. However, INCA-N is unable to model such decoupling phenomena.

7. Acknowledgement

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