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Technical Note: Alternative in-stream denitrification equation for the INCA-N model

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Abstract

The Integrated Catchment model for Nitrogen (INCA-N) is a semi-distributed, process based model that has been used to model the impacts of land use, climate, and land management changes on hydrology and nitrogen loading. An observed problem with the INCA-N model is reproducing low nitrate-nitrogen concentrations during the summer growing season in some catchments. In this study, the current equation used to simulate the rate of in-stream denitrification was replaced with an alternate equation that uses a mass transfer coefficient and the stream bottom area. The results of simulating in-stream denitrification using the two different methods were compared for a 9 month simulation period of the Yläneenjoki catchment in Finland. The alternate equation (Nash–Sutcliffe efficiency = 0.59) simulated concentrations during the growing season that were closer to the observed concentrations than the current equation (Nash–Sutcliffe efficiency = 0.47). The results of this work promote the incorporation of the alternate equation into the model for further testing.

1 Introduction

Catchment scale nutrient models can be used to predict the effect of changing land use and climate on nutrient export. The Integrated Catchment model for Nitrogen (INCA-N) is a catchment scale model that simulates both hydrology and mineral nitrogen processes (Wade et al., 2002; Whitehead et al., 1998). INCA-N has been applied to many European catchments, but one problem has been the overestimation of nitrate-nitrogen (NO_3-N) concentrations during the summer growing season (Jarvie et al., 2002; Rankinen et al., 2006). It is assumed that the current equations used in INCA-N to model in-stream denitrification also take into account other retention mechanisms (O'Shea and Wade, 2009), but other results show that a retention process such as macrophyte uptake is not accurately represented by the current equations for in-stream denitrification (Jarvie et al., 2002; Rankinen et al., 2006, 2013). There is also the potential for the overestimation of NO_3-N concentrations by the model caused by inaccuracies in the mass of nitrogen added to the stream through groundwater flow (Wade et al., 2006, 2008).

Birgand et al. (2007) proposed the use of a mass transfer coefficient (ρ) to quantify the in-stream NO_3-N retention in their extensive review of in-stream denitrification in agricultural catchments. The mass transfer coefficient multiplied by the NO_3-N concentration corresponds to the mass of nitrogen that would be removed from the water above a certain area of stream bed during a defined period of time. Birgand et al. (2007) recommended that the mass transfer coefficient be used in streams with NO_3-N concentrations above $1\,\mathrm{mg\,L^{-1}}$ based on the premise that above this threshold, the concentration gradient would be in a downward direction in accordance with the mass transfer coefficient theoretical application. The goal of this work was to test the equations proposed by Birgand et al. (2007) to determine their effectiveness in improving the INCA-N simulation of in-stream NO_3-N concentrations in the growing season of temperate and boreal climates.

2 Methods

2.1 In-stream mass balance of NO_3-N as implemented in the INCA-N model

The INCA-N model is a dynamic model that uses a mass balance approach to track the movement of mineral nitrogen in a catchment (Wade et al., 2002; Whitehead et al., 1998). Wade et al. (2002) described the equations for in-stream denitrification that have been used in the model since version 1.6. INCA-N model version 1.11.10 was used in this study.

Equation (1) shows how the mass of nitrogen removed through in-stream denitrification is calculated in the INCA-N model:

$$m_{\mathrm{INCA}} = \frac{R_{\mathrm{n}} C_{1,t-1} V}{1000} \tag{1}$$

where m_{INCA} is the total mass of nitrogen removed through in-stream denitrification in a single reach ($\mathrm{kg\,N\,day^{-1}}$), R_{n} is the temperature adjusted in-stream denitrification rate ($\mathrm{day^{-1}}$), $C_{1,t-1}$ is the in-stream $\mathrm{NO_3}$-N concentration on the previous day ($\mathrm{mg\,L^{-1}}$), and V is the volume of water stored in the reach ($\mathrm{m^3}$).

The denitrification rate (R_{n}) is temperature dependent, so it varies daily. The relation between temperature and the denitrification rate in the INCA-N model are shown in Eq. (2):

$$R_{\mathrm{n}} = 1.047R^{(T-20)} \tag{2}$$

where R is the process rate before temperature adjustment ($\mathrm{day^{-1}}$) and T is the in-stream water temperature (°C).

In the model, the water temperature is assumed to be the same as the air temperature, but a minimum water temperature is defined as a model input. In this simulation, the water temperature was not allowed to drop below 0 °C.

Equation (3) describes the in-stream mass balance calculations for $\mathrm{NO_3}$-N used in INCA-N:

$$\frac{\mathrm{d}m_{\mathrm{r}}}{\mathrm{d}t} = m_{\mathrm{in}} - \frac{Qm_{\mathrm{r},t-1} \times 86\,400}{V} - m_{\mathrm{INCA}} + \frac{R_{\mathrm{i}}C_{2,t-1}V}{1000} \tag{3}$$

where m_{r} is the mass of $\mathrm{NO_3}$-N stored in the stream reach (kg), m_{in} is the $\mathrm{NO_3}$-N input mass from upstream and non-point sources in the watershed ($\mathrm{kg\,N\,day^{-1}}$), Q is the reach discharge ($\mathrm{m^3\,s^{-1}}$), R_{i} is the temperature adjusted in-stream nitrification rate ($\mathrm{day^{-1}}$), and $C_{2,t-1}$ is the in-stream $\mathrm{NH_4}$-N concentration on the previous day ($\mathrm{mg\,L^{-1}}$).

2.2 Estimation of in-stream denitrification using the mass transfer coefficient

Equation (4) was used to calculate the mass of nitrogen removed by denitrification using the mass transfer coefficient and the stream bottom area. Equation (4) was adapted from Birgand et al. (2007). The m_{INCA} in Eq. (3) was replaced with the m_{alt} value to model the in-stream NO_3-N mass balance:

$$m_{\mathrm{alt}} = \frac{\rho_{\mathrm{n}} A C_{1,t-1}}{1000} \tag{4}$$

where m_{alt} is the total mass of nitrogen removed via in-stream denitrification in a single reach calculated based on the mass transfer coefficient and the stream bottom area ($\mathrm{kg\,N\,day^{-1}}$), ρ_{n} is the temperature adjusted mass transfer coefficient for NO_3-N removal through denitrification ($\mathrm{m\,day^{-1}}$), A is the stream bottom area of the reach ($\mathrm{m^2}$).

The mass transfer coefficient (ρ) is temperature dependent and is adjusted to temperature variations using an equation similar to Eq. (2). The assumption that the water temperature never drops below 0 °C was maintained for the mass transfer coefficient.

2.3 Model calibration

The alternate equation was tested on a simulation of the upper reaches of the River Yläneenjoki from April 2004 through December 2004. This period was chosen because it had a number of samples with low NO_3-N concentrations that were not adequately simulated after calibration of the model. The Yläneenjoki catchment is located in southwestern Finland and drains to Lake Pyhäjärvi. The model was applied to the portion of the river upstream of the Peräsuonoja monitoring station (Lepistö et al., 2008) to test the alternate equation. This sub-catchment has an area of 20.08 $\mathrm{km^2}$ with 28 % of the land being in agricultural production. The main reach of the River Yläneenjoki has a length of 4000 m in the modeled sub-catchment.

The hydrology portion of the model was calibrated first, followed by the nitrogen portion of the model using the methods described in Granlund et al. (2004) and Etheridge et al. (2013). The hydrology portion of the model was calibrated to continuous flow data at the Vanhakartano monitoring station, which is near the mouth of the river at Lake Pyhäjärvi (Lepistö et al., 2008; Etheridge et al., 2013), by adjusting the flow velocity parameters and time constants for the soil and groundwater zones. The nitrogen portion of the model was calibrated such that the in-stream nutrient concentrations followed the dynamics of the observed concentrations and were of similar magnitude. This was done by adjusting the nutrient process rates in the model. Data available related to nitrogen process rates ranging from fertilizer application data to rates of denitrification measured experimentally were used to reduce uncertainty in model results. More details about the Yläneenjoki Catchment and the model calibration can be found in Etheridge et al. (2013).

The in-stream denitrification and nitrification are the final two processes that alter nitrogen in the INCA-N model, so it was possible to change the in-stream denitrification calculations without changing the results from any other portion of the model. The order of calculations in INCA-N allowed the alternate equation calculations to be completed using a spreadsheet instead of altering the model code. Simulations with the alternate in-stream denitrification equation were done using Excel 2007 (Microsoft, Redmond, WA, USA). Equation 3 is the in-stream mass balance equation for NO_3-N in the model. The input mass of NO_3-N (m_{in}), the reach discharge (Q), the reach volume (V), and the mass of nitrogen that is nitrified in the reach are all outputs of the model. These model outputs were taken directly from the calibrated model and were not altered in this work. The primary change that was made was replacing m_{INCA} with m_{alt} in Eq. (3), which changes the concentration of NO_3-N in the stream.

To make the calculations using the alternate equation, the stream bottom area (A) of the modeled reach was estimated using ArcGIS (ESRI, Redlands, CA, USA). The main sources of data were a raster map (1 m resolution) of all of the water areas in Finland and a map showing the streamline of the modeled reach. A buffer was created around the modeled streamline using the analysis tools in ArcGIS. All of the water area from the raster map located within this buffer was considered the stream bottom area input to the model. The stream bottom area used in this simulation is 20 000 m^2. This method may overestimate the stream bottom area of the primary reach as it includes both the stream bottom and the banks in the projected area. This error was considered reasonable because the entire stream bottom in the catchment was not included, but denitrification and other retention processes occur in these tributaries that feed the main channel.

Assuming a constant stream bottom area throughout the modeling period was not an ideal representation of the physical system because the stream width (i.e. submerged width of the stream) will increase with increasing depth and flow. This simplifying assumption was made so that extensive collection of channel dimensions was not required and model complexity was not further increased. The wetted stream bottom area in natural streams is dynamic, but increasing the wetted area does not necessarily increase denitrification during periods of higher flow due to the reduction in residence time. As stream flow and depth increase, the amount of time that NO_3-N rich water would be exposed to sites suitable for denitrification decreases, so an increase in the actual wetted stream bottom area does not always indicate an increased removal of NO_3-N via denitrification. Having a constant stream bottom area in the model may compensate for the effect of water residence time on in-stream denitrification.

When using the alternate equation to calculate the mass of nitrogen removed from the system through in-stream denitrification, the mass transfer coefficient (ρ) was the only model input that was changed in the calibration process. An initial ρ was chosen based on values found in published results of many previous studies (Birgand et al., 2007). The calibration results were evaluated based on visual comparison to the observed data, the R^2 value, and the Nash–Sutcliffe (NS) efficiency. An NS efficiency greater than zero indicates that the model output is better than using the mean of the observed data (Nash and Sutcliffe, 1970). The ρ was adjusted to produce simulated NO_3-N dynamics which most closely followed the dynamics of the observed concentrations along with acceptable goodness-of-fit values.

3 Results and discussion

The outputs from the INCA-N model were compared to the results obtained using the alternate in-stream denitrification equation in Fig. 1. Based on visual inspection there was an improvement in the simulation of the observed NO_3-N concentrations that were below 1 mg L^{-1} using the alternate equation. For concentrations above 1 mg L^{-1} the results were mixed with each equation modeling certain observed concentrations better than the other. The primary time when the current INCA-N equation performed better than the alternate equation was in September. For the first two observed concentrations in September (1.2 and 4.0 mg L^{-1}), the alternate equation underestimated the observed concentrations and the INCA-N model was close to the observed values. Both of the equations underestimated the third observed concentration (6.3 mg L^{-1}) in September. A continuous record of NO_3-N would improve this analysis as the modeled dynamics of events, such as the one in mid-July, could be compared to the observed dynamics. The alternate equation simulated less nitrogen removal via denitrification than the INCA-N model during periods of high flow in April and December as indicated by the higher concentrations. Although the differences in concentrations appear to be small, they are important in the nutrient budget as the greatest fluxes occur during periods of high flow. The higher simulated NO_3-N values during these times produced better results than the simulations done using the current equations in INCA-N.

These results may show how important in-stream denitrification was compared to other NO_3-N transport and transformation processes during each season. During the summer period when the flow was low, the difference in NO_3-N prediction was the greatest between the current INCA-N model results and the alternate equation. From mid-May until the end of August, the alternate equation produced lower simulated NO_3-N concentrations than the equation currently used in INCA-N. At these times, uncertainty associated with all other parameter estimates may have played a lower role because of the quasi-steady state condition of low flow. Definite improvement of the model predictions at this time of the year may then be attributed to a better method of predicting in-stream retention. In other portions of the year other processes, such as leaching, played a primary role in determining the in-stream NO_3-N concentration, so it was more difficult to evaluate different methods of simulating in-stream denitrification.

Using the alternate equation improved the goodness-of-fit of the modeled results when compared to the observed concentrations. The original INCA-N equation produced a R^2 value of 0.52 and a NS of 0.47 when comparing the observed NO_3-N concentrations to the simulated concentrations. The alternate equation using the mass transfer coefficient produced 0.59 for both the R^2 and NS values. The improved goodness-of-fit values show the improved estimation of NO_3-N concentrations during the summer growing season by the alternate equation.

The rate of in-stream denitrification in the INCA-N model was 0.145 day^{-1}. This resulted in a total nitrogen removal due to in-stream denitrification of 2600 kg for the 9 month modeling period. This was equivalent to 17 % of the N that entered the stream being retained by in-stream processes. A mass transfer coefficient of 0.4 m day^{-1} was used in the alternate equation as it produced the best results through calibration. The 9 month nitrogen removal via in-stream denitrification was 2100 kg or 14 % of the total N that entered the stream for the alternate equation. The mass of nitrogen removed through denitrification was lower using the alternate equation because it did not simulate as much nitrogen removal during periods of high flow as can be seen by the higher NO_3-N concentrations at the end of the simulation period. The lower in-stream retention simulated by the alternate equation was closer to values of between 5 and 15 % that have been estimated in Finnish catchments (Lepistö et al., 2006; Martikainen et al., unpublished). The mass transfer coefficient of 0.4 m day^{-1} used in this model application was within the range of plausible values based on the review by Birgand et al. (2007), though most of the values in the review were below 0.3 m day^{-1}. One potential reason the mass transfer coefficient was higher in the model application than in field experiments was an underestimate of the stream bottom area. Recall, the stream bottom area was estimated only for the main reach modeled in INCA-N. It did not include the entire stream bottom area in the whole catchment. In-stream denitrification was occurring throughout the catchment in the many streams and drainage ditches that feed the main river channel. An increased stream bottom area would have reduced the mass transfer coefficient and produced similar results in the model. The assumption of a constant stream bottom area did not cause extreme peaks in NO_3-N concentrations during periods of high flow or extremely low NO_3-N concentrations during periods of low flow in the model calibration (Fig. 1), so this assumption appeared to be acceptable.

Using the alternate equation in INCA-N may improve the modeling results, but may not be the best representation of the natural processes that are occurring. It was possible that the overestimation of NO_3-N concentrations during the low flow summer period was also influenced by the groundwater storage of NO_3-N being modeled incorrectly (Wade et al., 2006, 2008). Further investigation is required into the influence of groundwater flow on in-stream NO_3-N concentrations and how this is modeled.

4 Conclusions

Although Birgand et al. (2007) recommended using the mass transfer coefficient when the NO_3-N concentrations were greater than $1\,\mathrm{mg\,L^{-1}}$, it appears that the alternate equation, using the mass transfer coefficient, simulates in-stream denitrification during low flow and low NO_3-N concentration conditions better than the current equations used in the INCA-N model. It was possible that a downward flux of NO_3-N continued to occur at concentrations below $0.5\,\mathrm{mg\,L^{-1}}$ and the alternate equation was still valid in this catchment. The impact of using the alternate equation during periods of higher flow and concentrations above $1\,\mathrm{mg\,L^{-1}}$ needs further evaluation in catchments that have more observation points.

An added input that is not easily defined, is not generally thought of as a model improvement. One drawback of using the mass transfer coefficient alternate equation in the INCA-N model is it requires an added input of stream bottom area. An improved simulation of in-stream NO_3-N retention during the summer growing season should promote the addition of model complexity. Using such a short period of time to test the use of the proposed in-stream denitrification equation is not as accurate as doing a multiple year calibration in the model, but this work provides evidence that the mass transfer coefficient equations should be considered as an alternate method of modeling the in-stream denitrification in the INCA-N model.

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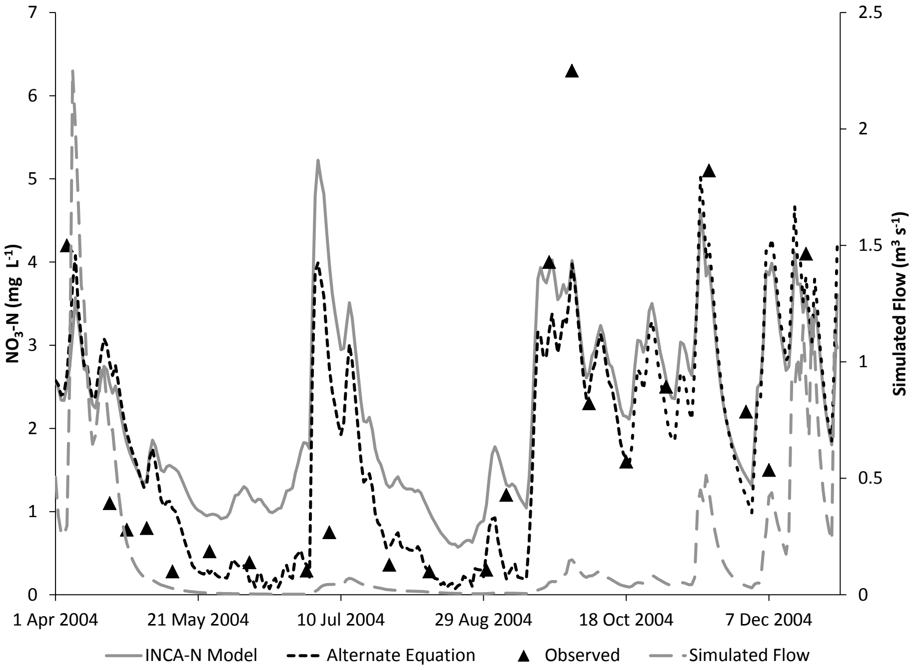

Fig. 1. Graph comparing the INCA-N model results to the results with the alternate equation.

HESSD

10, 14557–14569, 2013

Title Page
Abstract | Introduction
Conclusions | References
Tables | Figures
◀◀ | ▶▶
◀ | ▶
Back | Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion