Nitrogen Module: Principles and Governing Equations

1 Overview

We implement a lumped, daily-time-step nitrogen (N) module coupled to simulated streamflow. The module tracks three conceptual pools—ammonium (NH_4^+), nitrate (NO_3^-), and organic nitrogen (OrgN)—and represents (i) external inputs linked to hydrologic forcing, (ii) plant uptake, (iii) mineralization, (iv) temperature-modulated losses, and (v) hydrologic export. A first-order reservoir produces lagged NO_3^- signals at the outlet.

2 State Variables and Fluxes

Let $N_{\mathrm{NH4}}(t)$, $N_{\mathrm{NO3}}(t)$, $N_{\mathrm{Org}}(t)$ be pool masses (e.g., mg N m^{-2} or kg N ha^{-1}). Daily streamflow $Q(t)$ is provided by the HBV component. Temperature $T(t)$ drives biological rates.

External N input linked to flow:

$$I_{\mathrm{NH4}}(t) = \gamma Q(t), \qquad I_{\mathrm{NO3}}(t) = \gamma Q(t), \qquad I_{\mathrm{Org}}(t) = 1.5\,\gamma Q(t),$$

Vegetation activity index $V(t)$ (logistic with thermal optimum) modulates uptake:

$$V(t) = \frac{1}{1 + \exp[-0.5\,(T(t) - 15)]}.$$

A temperature modifier adjusts reaction/exit rates:

$$f_T(t) = \exp\left[\beta\,(T(t) - 10)\right],$$

where β controls temperature sensitivity.

3 Process Representations

(a) Plant uptake

$$U_{\mathrm{NH4}}(t) = k_{\mathrm{up}} V(t) N_{\mathrm{NH4}}(t), \qquad U_{\mathrm{NO3}}(t) = k_{\mathrm{up}} V(t) N_{\mathrm{NO3}}(t).$$

(b) Mineralization (OrgN → inorganic N)

$$M_{\text{Org}}(t) = k_{\text{dec}} N_{\text{Org}}(t).$$

Partitioning:

$$\Delta N_{\text{NH4}}^{\text{min}} = 0.2 M_{\text{Org}}(t), \quad \Delta N_{\text{NO3}}^{\text{min}} = 0.3 M_{\text{Org}}(t).$$

(c) Temperature-modulated hydrologic losses

$$L_{\text{NH4}}(t) = \alpha_{\text{NH4}} Q(t) f_T(t), \quad L_{\text{NO3}}(t) = \alpha_{\text{NO3}} Q(t) f_T(t), \quad L_{\text{Org}}(t) = \alpha_{\text{Org}} Q(t) f_T(t).$$

4 Pool Mass Balances (explicit Euler, daily)

$$\begin{aligned}
N_{\text{NH4}}(t+1) &= \max\{0, N_{\text{NH4}}(t) + I_{\text{NH4}}(t) + \Delta N_{\text{NH4}}^{\text{min}} - U_{\text{NH4}}(t) - L_{\text{NH4}}(t)\}, \\
N_{\text{NO3}}(t+1) &= \max\{0, N_{\text{NO3}}(t) + I_{\text{NO3}}(t) + \Delta N_{\text{NO3}}^{\text{min}} - U_{\text{NO3}}(t) - L_{\text{NO3}}(t)\}, \\
N_{\text{Org}}(t+1) &= \max\{0, N_{\text{Org}}(t) + I_{\text{Org}}(t) - M_{\text{Org}}(t) - L_{\text{Org}}(t) + 0.1\}.
\end{aligned}$$

5 Outlet Nitrate with Transport Lag

Instantaneous NO_3^- export $E_{\text{NO3}}(t) = L_{\text{NO3}}(t)$ is routed through a first-order linear reservoir:

$$Y_{\text{NO3}}(t) = (1-\lambda) Y_{\text{NO3}}(t-1) + \lambda E_{\text{NO3}}(t).$$

6 Parameters and Initial Conditions

$$\Theta = \{\alpha_{\text{NH4}},\ \alpha_{\text{NO3}},\ \alpha_{\text{Org}},\ k_{\text{up}},\ k_{\text{dec}},\ \beta,\ \gamma,\ N_{\text{NH4}}(0),\ N_{\text{NO3}}(0),\ N_{\text{Org}}(0),\ \lambda\}.$$

Typical bounds (used in calibration):

- α: [1e−4, 5e−2]
- k_{up}: [1e−3, 1e−1]
- k_{dec}: [1e−4, 2e−2]
- β: [0,1]
- γ: [0,0.1]
- $N(0)$: [0.1,50]
- λ: [0.01,0.5]

7 Coupling, Numerics, and Calibration

- **Coupling:** $Q(t)$ and $T(t)$ are provided by the hydrologic component (HBV). External N inputs scale with $Q(t)$.
- **Time stepping:** explicit Euler, daily. Non-negativity is enforced by truncation.
- **Objectives:** goodness-of-fit to observed stream NO_3^- using NSE or KGE, optionally MSE; flow is calibrated first, then N parameters are optimized conditional on simulated flow.
- **Identifiability:** γ, α_{NO3}, and λ may be correlated through their joint control on timing and magnitude; β interacts with seasonal $V(t)$.

8 Assumptions and Limitations

This is a reduced-form, lumped representation. Nitrification/denitrification are not explicitly separated; mineralization is a single first-order process with fixed partitioning. The first-order routing is a pragmatic proxy for in-stream and near-stream lags. Despite its simplicity, the structure captures primary controls of seasonal uptake, temperature, hydrologic export, and transport delay.

Symbol and Parameter Glossary

- Q(t): streamflow (driver)
- T(t): temperature (driver)
- V(t): vegetation activity index
- f_T(t): temperature modifier
- α_NH4, α_NO3, α_Org: hydrologic loss coefficients
- k_up: plant uptake rate
- k_dec: mineralization rate
- β: temperature sensitivity
- γ: external input coefficient
- N_NH4(0), N_NO3(0), N_Org(0): initial pools
- λ: routing/lag parameter
- Y_NO3(t): lagged NO_3^- signal at outlet