Process-Based Nitrification Module (Del Grosso–type Formulation)

1. Overview

We implement a process-based nitrification module following Del Grosso–type response functions. The daily nitrification rate is computed as a **potential term** driven by ammonium availability and humus decomposition, **modulated multiplicatively** by soil water-filled pore space (WFPS), temperature, and pH response functions. Soil-specific coefficients allow heterogeneity across soil classes. This nitrification flux is coupled to the nitrogen pools and hydrologic drivers defined elsewhere in the model.

2. Governing Formulation

2.1 Potential Term

Let $N_{\mathrm{NH4}}(t)$ be the $\mathrm{NH_4^+}$ pool and $H_{\mathrm{dec}}(t)$ the daily amount of N released from humus decomposition. The potential (unlimited) nitrification driver is

$$B(t) = k_1 \, H_{\mathrm{dec}}(t) + k_{\max} \, N_{\mathrm{NH4}}(t),$$

where k_1 and $k_{\max}$ are rate coefficients.

2.2 Environmental Limitation Functions

(a) Water limitation (WFPS):

$$F_w(w) = \left(\frac{w - c_1}{c_0 - c_1} \right)^{c_3 \frac{(c_1 - c_0)}{(c_0 - c_2)}} \left(\frac{w - c_2}{c_0 - c_2} \right)^{c_3},$$

with w the water-filled pore space (WFPS) and c_0, c_1, c_2, c_3 empirical shape parameters.

(b) Temperature limitation:

$$F_T(T) = \left(\max\left\{0,\ \frac{c_1 - T}{c_1 - 25}\right\}\right)^{c_2} \exp\left(\frac{c_2}{c_3}\left[1 - \left(\max\{0, \tfrac{c_1 - T}{c_1 - 25}\}\right)^{c_3}\right]\right),$$

where T is soil temperature (°C) and c_1, c_2, c_3 control the curve shape and optimum.

(c) pH limitation:

$$F_{\mathrm{pH}}(\mathrm{pH}) = \min\left\{1,\ c_1 + \frac{c_2}{\pi}\arctan\big(\pi c_3(\mathrm{pH} - c_0)\big)\right\}.$$

2.3 Nitrification Rate

The daily nitrification flux (mass per area per day) is

$$R_{\mathrm{nit}}(t) = \eta\ B(t)\ F_w\big(w(t)\big)\ F_T\big(T(t)\big)\ F_{\mathrm{pH}}\big(\mathrm{pH}\big),$$

where η is a scaling factor (see below). In implementation:

$$R_{\mathrm{nit}}(t) = \eta\ \left(k_1\, H_{\mathrm{dec}}(t) + k_{\max}\, N_{\mathrm{NH4}}(t)\right)\ F_w\, F_T\, F_{\mathrm{pH}}.$$

Parameters and Defaults

- **Kinetics:** k_1 (humus-derived), $k_{\max}$ (NH_4^+-derived) — soil-specific.
- **WFPS response:** $c_0 = 0.5$, $c_1 = 0.0$, $c_2 = 1.5$, $c_3 = 4.5$.
- **Temperature response:** $c_1 = -5.0$, $c_2 = 7.0$, $c_3 = 4.5$.
- **pH response:** $c_0 = 5.0$, $c_1 = 0.56$, $c_2 = 1.0$, $c_3 = 0.45$.
- **Scale factor:** $\eta = 1000$ (unit/scale alignment with model outputs).
- **Soil heterogeneity:** soil-specific parameter sets (e.g., $k_1, k_{\max}$, porosity, depth, pH) selected by soil ID.

Variable and Function Glossary

- $N_{\mathrm{NH4}}(t)$: ammonium pool.
- $H_{\mathrm{dec}}(t)$: daily N released from humus decomposition.
- $w(t)$: water-filled pore space (WFPS).
- $T(t)$: soil temperature (°C).
- pH: soil acidity/alkalinity.

- $F_w, F_T, F_{\mathrm{pH}}$: environmental limitation functions.
- $R_{\mathrm{nit}}(t)$: nitrification rate (flux).
- η: scale factor.