Process-Based Nitrification Module (Parton–type Formulation)

1. Overview

We implement a process-based nitrification module following Parton–type response functions. The daily nitrification rate combines a **humus-derived source** from decomposition and an **NH_4^+-driven potential**, **modulated multiplicatively** by environmental scalars for soil moisture (WFPS), temperature, and pH. Soil- and layer-specific parameters (e.g., porosity, depth, pH, bulk density) represent heterogeneity across soils. Unit conversions are applied between mass- and area-based forms to maintain consistency with the rest of the model.

2. Governing Formulation

2.1 Sources (humus- and NH_4^+-driven)

Let $H_{\mathrm{dec}}(t)$ be the daily nitrogen released from humus decomposition (mass units), and $N_{\mathrm{NH4}}(t)$ the ammonium pool. A fraction of decomposed humus contributes directly to nitrification after conversion to concentration units; an NH_4^+-driven term provides the potential substrate for nitrification:

$$S_h(t) \;=\; f_h\, C_{\mathrm{humus,dec}}(t), \qquad S_n(t) \;=\; k_{\max}\, C_{\mathrm{NH4}}(t),$$

where $f_h \approx 0.2$ (humus-to-nitrification fraction), $k_{\max}$ is the maximum nitrification rate constant, and $C_{\mathrm{humus,dec}},\ C_{\mathrm{NH4}}$ are concentrations (e.g., mg g^{-1}) obtained from pool masses using bulk density and layer depth.

2.2 Environmental Limitation Functions

(a) Water limitation (WFPS):

$$F_w(w) = \left(\frac{w-b}{a-b}\right)^{d\,\frac{(b-a)}{(a-c)}} \left(\frac{w-c}{a-c}\right)^{d},$$

where w is water-filled pore space, and a, b, c, d are shape parameters.

(b) Temperature limitation:

$$F_T(T) = a + b\,\exp(cT),$$

with coefficients (a, b, c) controlling baseline, amplitude, and sensitivity.

(c) pH limitation:

$$F_{\mathrm{pH}}(\mathrm{pH}) = a + \frac{1}{\pi}\arctan(\pi b(c + \mathrm{pH})),$$

with parameters (a, b, c) shaping the curve.

2.3 Nitrification Rate

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

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

where η is a scale/units conversion factor to reconcile concentration- to area-based flux.

Parameters and Defaults

- **Kinetics:** $f_h = 0.2$, $k_{\max}$ (soil-specific).
- **WFPS response:** $a = 0.4, b = 1.7, c = -0.007, d = 3.22$.
- **Temperature response:** $a = -0.06, b = 0.13, c = 0.07$.
- **pH response:** $a = 0.56, b = 0.45, c = -5.0$.
- **Bulk density:** default 1.52 g cm^{-3}.
- **Scale factor:** $\eta = 1000$ (to align with model units).
- **Soil heterogeneity:** soil-specific $k_{\max}$, porosity, depth, pH, humus decay rate, bulk density.

Variable and Function Glossary

- $N_{\mathrm{NH4}}(t)$: ammonium pool.
- $H_{\mathrm{dec}}(t)$: daily N released from humus decomposition.
- $C_{\mathrm{NH4}}, C_{\mathrm{humus,dec}}$: concentrations (mg g^{-1}).

- $w(t)$: 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 flux (mass per area per day).
- η: scale/units conversion factor.