Process Rate Estimator

A modeling side-hustle for the ETH group sustainable agroecosystems

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1 Introduction

Denitrification is the natural process by which nitrate (NO_3^-) in the soil are converted by bacteria into nitrous oxide (N_2O) or pure nitrigen (N_2). The latter is called *total denitrification* — the full process described in Equation 1 takes place.

$$\mathrm{NO_3}^- \xrightarrow[\text{reductase}]{\text{Nitrate}} \mathrm{NO_2}^- \xrightarrow[\text{reductase}]{\text{Nitrite}} \mathrm{NO} \xrightarrow[\text{reductase}]{\text{Nitrite oxide}} \mathrm{N_2O}^- \xrightarrow[\text{reductase}]{\text{Nitrous oxide}} \mathrm{N_2} \tag{1}$$

Denitrification occurs in conditions where oxygen is limited, such as waterlogged soils. It is part of the nitrogen cycle, where nitrogen is circulated between the atmosphere, organisms and the earth.

2 Formal model description

The diffusion fluxes between soil increments are described by Frick's law (Equation 2).

$$F_{\text{calc}} = \frac{dC}{dZ} D_{\text{s}} \rho \tag{2}$$

Here, D_s is the gas diffusion coefficient, ρ is the gas density of N_2O, and $\frac{dC}{dZ}$ is the N_2O concentration gradient from lower to upper depth.

The gas diffusion coefficient D_{s} was calculated according Equation 3 as established by Millington and Quirk in 1961.[1]

$$D_{\text{s}} = \left(\frac{\theta_w^{\frac{10}{3}} + D_{\text{fw}}}{H} + \theta_a^{\frac{10}{3}} \times D_{\text{fa}} \right) \times \theta_T^{-2} \tag{3}$$

Here, H represents a dimensionless form of Henry's solubility constant (H') for N_2O in water at a given temperature. The constant H for N_2O is calculated as follows:

$$H = \frac{8.5470 \times 10^5 \times \exp \frac{-2284}{\mathrm{T}}}{\mathrm{R} \times \mathrm{T}} \tag{4}$$

Here, R is the gas constant, and T is the temperature (T = 298 K).

References

1. Millington, R. & Quirk, J. Permeability of porous solids. *Transactions of the Faraday Society* **57**, 1200–1207 (1961).