

Process Rate Estimator

A modeling side-hustle for the ETH group sustainable agroecosystems

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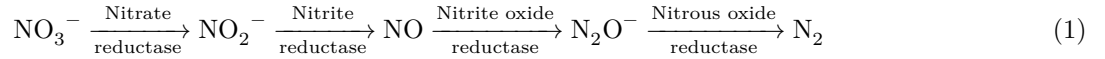
September 23, 2023

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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 nitrogen (N_2). The latter is called *total denitrification* — the full process described in Equation 1 takes place.



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).

$$F_{\text{calc}} = \frac{dC}{dZ} D_s \rho \quad (2)$$

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 fluxes are calculated based on N_2O concentration gradients between 105-135 cm, 75-105 cm, 45-75 cm, 15-45 cm, and 0-15 cm depth layers, and ambient air above the soil surface.

The gas diffusion coefficient D_s was calculated according Equation 3 as established by Millington and Quirk in 1961.¹

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

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:

$$H = \frac{8.5470 \times 10^5 \times \exp \frac{-2284}{T}}{R \times T} \quad (4)$$

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

D_{fw} was calculated according to Equation 5 as documented by Versteeg and Van Swaaij (1988).²

$$D_{\text{fw}} = 5.07 \times 10^{-6} \times \exp \frac{-2371}{T} \quad (5)$$

References

1. Millington, R. & Quirk, J. Permeability of porous solids. *Transactions of the Faraday Society* **57**, 1200–1207 (1961).
2. Versteeg, G. F. & Van Swaaij, W. P. Solubility and diffusivity of acid gases (carbon dioxide, nitrous oxide) in aqueous alkanolamine solutions. *Journal of Chemical & Engineering Data* **33**, 29–34 (1988).