



## Isotope fractionation factors of N<sub>2</sub>O production and reduction by denitrification: b. Modeling data from soil incubation under N<sub>2</sub>-free atmosphere

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Quantifying denitrification in arable soils is crucial in predicting the microbial consumption of nitrogen fertilizers as well as N<sub>2</sub>O emissions. Stable isotopologue analyses of denitrification substrates ( $\delta^{15}\text{N}_{\text{NO}_3}$ ,  $\delta^{18}\text{O}_{\text{NO}_3}$ ) and products ( $\delta^{15}\text{N}_{\text{N}_2\text{O}}$ ,  $\delta^{18}\text{O}_{\text{N}_2\text{O}}$  and  $\text{SP}_{\text{N}_2\text{O}}$  = Site Preference, i.e. difference in  $\delta^{15}\text{N}$  between the central and peripheral N positions of the asymmetric N<sub>2</sub>O molecule) can help to distinguish production pathways and to identify N<sub>2</sub>O reduction to N<sub>2</sub>. However, such interpretations are often ambiguous due to insufficient knowledge on isotopic fractionation mechanisms and wide differences in isotope fractionation factors determined by various studies for N<sub>2</sub>O production and reduction.

Here we present an original approach to determine fractionation factors associated with denitrification. This determination is based on simultaneous modeling of both reaction steps (N<sub>2</sub>O production and reduction) and comparison of the results with experimental data from a laboratory incubation experiment carried out under N<sub>2</sub>-free atmosphere. During the incubations N<sub>2</sub>O and N<sub>2</sub> concentrations were measured continuously, hence the reduced fraction ( $\text{N}_2/(\text{N}_2+\text{N}_2\text{O})$ ) was calculated directly from measured gas fluxes. Various modeling approaches have been applied to estimate the ranges of isotopic fractionation factors controlling the isotopic signatures of soil-emitted N<sub>2</sub>O. Initially, assumed isotope fractionation factors and the Rayleigh equations describing isotopic fractionation were used to calculate the theoretical  $\delta^{15}\text{N}$ ,  $\delta^{18}\text{O}$  and SP values for emitted N<sub>2</sub>O. Afterwards, the best fit fractionation factors for N<sub>2</sub>O production and reduction were determined by comparing modeled and measured values.

For two analyzed arable soils (clay and sandy loam), the isotopic fractionation factors were very consistent. For N<sub>2</sub>O production mean net isotope effects of  $\eta^{15}\text{N}_{\text{N}_2\text{O}-\text{NO}_3} \sim -41\text{‰}$ ,  $\eta\text{SP}_{\text{N}_2\text{O}-\text{NO}_3} \sim 2\text{‰}$  and  $\eta^{18}\text{O}_{\text{N}_2\text{O}-\text{H}_2\text{O}} \sim +40\text{‰}$  have been found. For N<sub>2</sub>O reduction mean net isotope effects of  $\eta^{15}\text{N}_{\text{N}_2-\text{N}_2\text{O}} \sim +1\text{‰}$ ,  $\eta\text{SP}_{\text{N}_2-\text{N}_2\text{O}} \sim -7\text{‰}$  and  $\eta^{18}\text{O}_{\text{N}_2-\text{N}_2\text{O}} \sim -5\text{‰}$  have been found. When compared to previous reports these results show significantly lower fractionation for  $\delta^{15}\text{N}$  and  $\delta^{18}\text{O}$  values during N<sub>2</sub>O reduction, which is most likely due to enhanced experimental approach that largely eliminates laboratory artifacts.