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Determination of nitrous oxide processes in soil from depth profiles of natural abundance stable isotope values by diffusion-reaction-fractionation modelling

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Analysing isotopocule values of nitrous oxide (N_2O) produced in soil can be used to distinguish N_2O production pathways and to quantify N_2O reduction to N_2. In the field, this is typically accomplished by analysing gas samples collected from closed chambers and calculating the isotopocule values of soil-emitted N_2O taking into account the fraction of atmospheric N_2O. Accuracy of this approach is often limited when N_2O fluxes are low, leading to small fraction of soil-derived N_2O in the chamber gas. To overcome this limitation, some studies used N_2O isotopocules of soil air, assuming that these reflected N_2O produced in soil (Gallarotti *et al.*, 2021, Zou *et al.*, 2014). However, this can lead to inaccurate results because (i) due to bi-directional diffusive gas exchange with the atmosphere, soil air is a mixture of soil-derived and atmospheric N_2O and (ii) isotopic fractionation during diffusive flux to the atmosphere leads to enrichment of residual N_2O in soil air. To evaluate these confounding factors and develop an approach to determine isotopocules of N_2O produced in soil from soil air samples, we compared surface fluxes of N_2O isotopocules determined by the closed chamber method (Lewicka-Szczebak et al. 2020) with gas probe data. Moreover, a diffusion-reaction model (Maier *et al.*, 2017, Well *et al.*, 2019) will be extended to include isotopic fractionation in order to determine isotopocule values of produced N_2O from soil air data. Scenarios varying in depth–dependent N_2O production and diffusivity will be analyzed. Results will show to which extent soil air and production values differ, which bias is obtained by using uncorrected soil air values, how well values can be corrected by modeling, and under which conditions soil air sampling might lead to better performance than closed chamber sampling. We expect that soil air sampling can lead to improved sensitivity for isotopocule values of soil-derived N_2O in certain cases, but correction of data is obligate to obtain useful results.

End Text

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