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Enhanced interpretation of N_2O isotopocule datasets with three dimensional modelling of simultaneous mixing and fractionation processes

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The isotopocule N_2O data (including N and O isotope values, but also the site specific N signature) are rich in information, but also challenging in their interpretation due to: (i) three dimensional isotope data, (ii) multiple potential N_2O production pathways, including at least four main processes (nitrification, bacterial and fungal denitrification and nitrifier denitrification), (iii) N_2O production and reduction processes occurring simultaneously. Therefore, advanced calculation approaches are necessary to deal with this complex case. The recently proposed calculation software for isotope FRActionation and Mixing Evaluation (FRAME) [1] allows source partitioning of different N_2O production pathways as well as estimation of the N_2O fraction reduced to N_2, based on all three isotope dimensions of N_2O. It applies Bayesian statistics (Markov Chain Monte Carlo) and provides probability distribution for the possible outcomes, taking into account the uncertainties associated both with measurements and natural variability.

This tool has been applied for interpretations of N_2O isotopocule datasets of field and experimental studies for soil and groundwater from the area of intensive organic fertilization in SW Poland. We have tested various strategies for enhancing the interpretation potential based on the N_2O isotopocule studies including: (i) increasing the $\delta^{15}N$ values of one mineral N pool (e.g. only nitrate or ammonium) in order to shift the overlapping mixing endmember ranges, (ii) lowering $\delta^{18}O$ of soilwater to better distinguish O-isotope exchange with soil water during denitrification. Some of the model outcomes were compared with independent methods (microbial gene expressiion and N_2/Ar method) and showed good agreements.

This modelling approach provides best results when the different mixing endmember ranges are precisely determined and do not overlap, which can be potentially attained by artificial manipulations of the substrates for particular N_2O production pathways.

References:

[1] Lewicki MP, Lewicka-Szczebak D, Skrzypek G. FRAME—Monte Carlo model for evaluation of the stable isotope mixing and fractionation. PLoS One. 2022;17(11):e0277204.