TimeFRAME - Time-resolved FRactionation And Mixing Evaluation based on isotope modeling of time series data

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Isotopic measurements of trace gases such as N_2O, CO_2 and CH_4 contain valuable information about production and consumption pathways. Quantification of the underlying pathways contributing to variability in isotopic timeseries can provide answers to key scientific questions, such as the contribution of nitrification and denitrification to N_2O emissions under different environmental conditions, or the drivers of multiyear variability in atmospheric CH_4 growth rate. However, there is currently no data analysis package available to solve isotopic production, mixing and consumption problems for timeseries data in a unified manner.

Here we present the TimeFRAME data analysis package for 'Time-resolved FRactionation And Mixing Evaluation'. We used Bayesian hierarchical models to solve production, mixing, and consumption contributions using multi-isotope timeseries measurements. Incorporation of temporal information reduced uncertainty and noise compared to model runs where data points were considered independent. Experiments with simulated data for $\delta^{15}N^{bulk}$ and $\delta^{15}N^{SP}$ of N_2O showed that model performance across all classes could be greatly improved by reducing uncertainty in model input data - particularly isotopic endmembers and fractionation factors. The addition of isotopic dimensions orthogonal to existing information could strongly improve results, for example clumped isotopes. The TimeFRAME package is available in R and can be used to evaluate both static and timeseries datasets, with flexible choice of the number and type of isotopic endmembers and the model set up allowing simple implementation for different trace gases.