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Bayesian end-member mixing analysis with explicit consideration of unobserved end-members and measurement uncertainty

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The identification of groundwater recharge sources and flow paths is key for sustainable groundwater management. Mixing ratios from different water sources are commonly estimated using end-member mixing analysis (EMMA).

Although the importance of the correct identification of the end-members and the influence of measurement uncertainty have been recognized in the literature, so far these uncertainties have only been partly represented in the model structure. EMMA assumes that conservative tracer concentrations of a water sample are represented solely by a mixture of samples from predefined end-members. However, even a careful selection of end-members (e.g. with PCA) cannot exclude the possibility of a contribution from an unknown, unmeasured end-member. Whenever such an additional end-member exists the standard model assumptions are violated and the resulting mixing ratios are biased.

We present a Bayesian extension of the EMMA with two novel features to deal with the aforementioned problems. For the estimation of the mixing ratios the presented model considers explicitly i) the measurement uncertainty of the tracer concentrations and ii) the possibility of an unknown *residual end-member*. Unlike the classical EMMA, this allows for extensive uncertainty quantification by providing the posterior distribution for all quantities. Not only the uncertainties of end-member mixing ratios can be expressed, but also the mixing ratio of the residual end-member and its tracer concentrations are quantified. Additionally, tracers with large measurement errors can be identified. Such extra information is valuable to design the experimental setup of future measurements. The model is also flexible regarding assumptions of the measurement uncertainties. For example absolute and relative errors or non-Gaussian distributions can be implemented readily.

We applied the model at a major water supply system in Switzerland to estimate mixing ratios between artificially infiltrated surface water and regional groundwater at several drinking water and observation wells. We used a set of tracers including ^{4}helium (He) analyzed on-site with a newly developed portable membrane-inlet mass spectrometry system. As an inert noble gas He serves as a very conservative tracer. The two selected end-members contribute together to at least 90% for 17 wells. For five wells, however, the model identified a substantial contribution (up to 45%) of an unknown residual end-member. This result can be used to confirm or revise the conceptual process understanding. The explicit consideration of measurement uncertainty enabled us also to quantify the benefits of using on-site ^{4}He measurements as a new tracer for estimating mixing ratios.

We belief that explicitly expressing assumptions about model structure deficits and measurement uncertainties has two main advantages: it protects from over-interpreting noisy data and it encourages the scientific community to discuss, challenge, and test different underlying model assumptions.