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Compensation of mass spectrometric interferences with the miniRUEDI portable mass spectrometer

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The miniRUEDI is a portable mass spectrometer system, which is widely used in environmental research[1,2] to study biogeochemical turnover and the origin, mixing and exchange of fluids. The miniRUEDI instruments are designed for on-site gas analysis during field work at remote locations and allow quantification of individual gas species in gaseous or aqueous matrices. The partial pressures of the gas species in a sample (e.g., He, Ar, Kr, N_2, O_2, CO_2, CH_4, etc.) are calibrated by peak-heights comparison relative to a reference gas with well known partial pressures.

However, depending on the target species and the composition of the analyzed gases, some ion-current peaks may result from overlapping signals from different species contributing to the ion-current at the same *m/z* ratio (e.g. $CH_4/O_2/N_2$ or $Ne/Ar/H_2O$). Such interferences need to be disentangled and compensated to allow accurate calibration of the gas partial pressures by ion-current peak-height comparison. We developed a tool that allows accurate compensation of such interferences by deconvolution the measured ion-current spectra in terms of the underlying spectra of the involved gas species.[3] The deconvolution yields the fractions of the ion-current contributions of the various gas species to a given ion-current peak and thereby accomplishes a substantial improvement of the analytical accuracy in situations where mass-spectrometric interferences cannot be avoided. Tests showed that the new tool allows accurate quantification of CH_4 and Ne at low abundances as typically observed in environmental fluids.[3]

(1) Brennwald et al. (2016), Environ. Sci. Technol. 50, 24, 13455-13463, DOI: 10.1021/acs.est.6b03669
(2) Gasometrix GmbH, Switzerland (www.gasometrix.com)
(3) Brennwald et al. (2020), MethodsX, 7, DOI: 10.1016/j.mex.2020.101038