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Two-Pronged Approach to Overcome Spectroscopically Interfering Organic Compounds with Isotopic Water Analysis

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The ability to measure the stable isotopes of hydrogen (dD) and oxygen (d18O) has become much more accessible with the advent of Cavity Ring-Down Spectroscopy (CRDS) laser optical devices. These small and inexpensive analyzers have led to a significant increase in the acquisition of data from a variety of studies in the fields of groundwater, watershed, and other water source applications.
However for some samples, such as those linked to fracking, mining, and other activities where higher than normal concentrations of organic materials are to be found, optical spectroscopy may require an adaptation from current methodologies in order to ensure data confidence. That is because CRDS is able to measure all the components within a spectral region – which will include the spectral characteristics of the isotopologues of water as well as the available features from interfering organic molecules. Although, at the first level, the information from the organic material provides spectral overlaps that can perturb the isotopic ratios, a more thorough review shows that these features are a source of information that will be inherently useful.
This presentation will examine the approaches developed within the past year to allow for more accurate analyses of such samples by optical methods. The first approach uses an advanced spectroscopic model to flag the presence of organic material in the sample. Signals from known interfering compounds (i.e. alcohols, ketones, aldehydes, short-chain hydrocarbons, etc.) are incorporated into the overall fit of the measured spectra used to calculate the concentration of the individual isotopes. The second approach uses physical treatment of the sample to break down the organic molecules into non-interfering species. The vaporized liquid or solid sample travels through a cartridge packed with an oxidation catalyst. The interfering organic molecules will undergo high temperature oxidation using O_2 present in the air carrier gas stream prior to isotopic measurement with CRDS. This approach is highly effective for organics at lower (< 5% v/v) concentrations and is promising to be extended to some higher concentration contamination as it was recently shown in our preliminary experiments.