Goldschmidt 2024 Abstract
https://doi.org/10.46427/gold2024.24691

Fingerprinting organic compounds in produced water: compound-class evaluation using ^{1}H-NMR

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The presence of unidentified organic compounds in produced water is a significant challenge for disposal, remediation, and reuse strategies. As produced water is the general term for any water recovered during petroleum drilling or extraction, the organic compound load in these waters is influenced by rock-water-hydrocarbon-microbe interactions as well as any fracking and drilling fluids used. The resulting produced water is very heterogeneous with respect to organic compound composition and concentration and often high in salinity. This chemical diversity complicates organic compound identification, which in turn makes assessment of environmental and health impacts and remediation strategies difficult. While some organic compounds can be identified via conventional solvent extraction and GC-MS methods, the composition of most of the organic carbon content is unknown, and therefore the reactivity and transport of these dissolved organic compounds in produced water is relatively unconstrained.

We have developed a method involving proton nuclear magnetic resonance (^{1}H-NMR) to determine compound-class level information about the organic compounds present in produced water samples. Using a set of produced water samples from the Black Warrior Basin (Alabama) coalbed methane play with varying salinity and total organic carbon content, we demonstrate that our procedure is relatively quick, requires minimal sample preparation, and can be performed on unaltered produced water, including samples with high salinity. The generated ^{1}H-HMR spectra provides a qualitative ‘fingerprint’ of the organic functional groups present in the sample, which can be used to evaluate the types of organic molecules present at the compound-class level. In general, aliphatic-type compounds were the most predominant, with carbohydrate/unsaturated and aromatic-type compounds being less abundant both in concentration and occurrence. This information can then be compared with the data from other produced water samples to identify geochemical trends, correlate with basin hydrology, compare within regions or between regions, or evaluate the efficacy of remediation methods. Ultimately, our goal is that this ‘fingerprinting’ method will be useful for identifying the biogeochemical processes that occur in hydrocarbon reservoirs as well as providing valuable information for produced water management, remediation, and health assessments.