Organic sulfur-bearing species as subsurface carbon storage vectors

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While there is much demand for negative CO_2 emission technologies [1], many research gaps are yet to be filled. To tackle climate change issues at scale, a combination of solution routes will be required. In this sense, could altered residual biomass be permanently sequestered in the subsurface, instead of returning its carbon content to the amosphere?

This work revisits mechanisms of natural sulfurization processes that form biologically refractory compounds, and investigates usage of these as substracts to generate water-soluble organic molecules. Such molecular vectors, could, in theory, be injected in shallow, saline, contaminated aquifers as a potential carbon sequestration method.

As model molecular libraries, sulfur-rich crude oils were analyzed with Fourier transform ion cyclotron resonance mass spectrometry to reveal molecular compositions of complex organosulfur compounds in such oils. A series of sulfurized compounds were detected, including $C_{20\text{-}28}$, C_{35} and C_{40} species with double bond equivalent values suggesting the occurrence of sulfurized lipids (steroids, hopanoids and carotenoids). Laboratory sulfurization reactions of lipid and carbohydrate standards [2], at various temperatures and time durations, were used to simulate natural sulfurization processes yielding products with up to 7 sulfur atoms within their structure. Modeled biodegradation resistance and water solubility estimates of the targeted vectors are presented. The conversion of S into SOx functional groups using mild oxidation reactions to increase water-solubility and assessment on the feasibility of such routes to negative emission technologies are the next steps in this study.

[1] Smith, P. *et al.* (2015) *Nature Climate Change* **6**, 42–50.
[2] Kok, M.D. *et al.* (2000) *Geochimica et Cosmochimica Acta* **64**, 2689–2699.