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Molecular dynamics of Organosulfur compounds in an oil sands pit lake via ESI FT-ICR MS: Implications for sulfur cycling in hydrocarbon-rich environments

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Base Mine Lake (BML), operated by Syncrude, is the first largescale commercial demonstration/application of water-capping technology in the oil sands industry intended for reclamation of fluid fine tailings. Sulfur containing organics are known to be associated with oil sands bitumen and sulfur containing naphthenic acids have been proposed as tracers of oil sands process water thus sulfur cycling may play an important role within this system. Both compound classes have the potential to be involved in biogeochemical cycling, particularly at the oxic/anoxic interface of the system where sulphate reduction can interface with sulfur oxidation. In this study, negative-ion mode electrospray ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI-FT-ICR-MS) was applied to characterize temporal changes in polar organosulfur compounds within this system from 2015 to 2023 at the epilimnion and hypolimnion with comparison to a nearby natural waterbody (BCR), an oil sands tailings pond (TP), and a ~30-year-old demonstration pond (DP). BML, TP, and DP are characteristically distinct from BCR. Compounds tentatively identified by chemical formula in BML, TP, and DP averaged ~11,000 of which ~30% were oxygenated organics and ~27% were oxygenated organosulfur compounds while BCR averaged ~6000 which consisted of ~40% oxygenated organics and ~20% oxygenated organosulfur compounds. At all sites O_xS_1 were the dominant organosulfur compounds making up ~16% of compounds at BCR and ~20% at BML, TP, and DP. OxS_2 compounds varied across sites (BCR: ~3%, BML: ~6%, TP: ~8%, and DP: ~4%). Within BML there appears to be a cyclic trend in the presence of higher mass O_xS_y compounds of carbon number > 25 that possess 3 to 6 oxygens. Additionally, highly oxygenated organosulfur compounds consisting of 8+ oxygens decrease over time. These trends appear to be present in the both the epilimnion and hypolimnion with the hypolimnion possessing fewer organosulfur compound classes in many of the years studied. These trends are continuing to be studied but currently suggest over time oxygen will continue to be consumed through sulfur oxidizing microbial processes in tandem with sulfur reducing bacterial metabolisms and that sulfur cycling may be an important consideration impacting the success of future pit lakes.