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Chemistry and Toxicology of Oil Sands Process Affected Water

By

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Oil Sands process-affected water (OSPW), produced during the extraction of bitumen in the surface-mining Oil Sands industry in Alberta, Canada, is acutely and chronically toxic to aquatic organisms. Organic compounds that are dissolved in the OSPW are responsible for most toxic effects, but knowledge of the specific chemicals that cause this toxicity, or their associated mechanism(s) of toxicity, is very limited. Due to the complexity of the dissolved organic fraction of OSPW, traditional bottom-up mixture toxicity prediction approaches are not practical. Therefore, a top-down approach to mixture toxicity predictions was developed, whereby accurate masses and not structures of chemicals are used for identification purposes by use of linear ion trap (orbitrap) ultrahigh resolution mass spectrometry. Using either solid phase micro-extraction (SPME) or solid-supported lipid membranes (SSLM), accurate masses were assigned a measured estimate of bioaccumulation. A narcosis mode of action was assumed and the target-lipid model of Di Toro *et al.*, (2000) was applied for toxicity predictions by use of measured bioaccumulation estimates of the individual accurate masses. The toxicity of the mixture was predicted assuming strict additivity. A model developed using a combination of the SPME and SSLM methods, where preference was given to SSLM bioaccumulation estimates, compared best with LC_{50} estimates from 96-hr acute lethality assays with embryos of fathead minnows (*Pimephales promelas*). Model predictions were within 4-fold of observed toxicity for 75% of samples and within 8-fold for all tested samples, well within inter-laboratory variability. In addition, the toxic unit approach was used to investigate the contribution of chemical classes of concern to toxicity of the mixture. This work highlights improvements made in the development of a model for predicting the acute toxicity of fractions and samples of OSPW to early-life stages of fathead minnow.

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