Supplementary Information (SI) for Environmental Science: Processes & Impacts.

Supplementary Information

Depletion rates of O_2-naphthenic acids from oil sands process-affected water in wetland microcosms

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Figures: 3

Tables: 3

Pages: 6

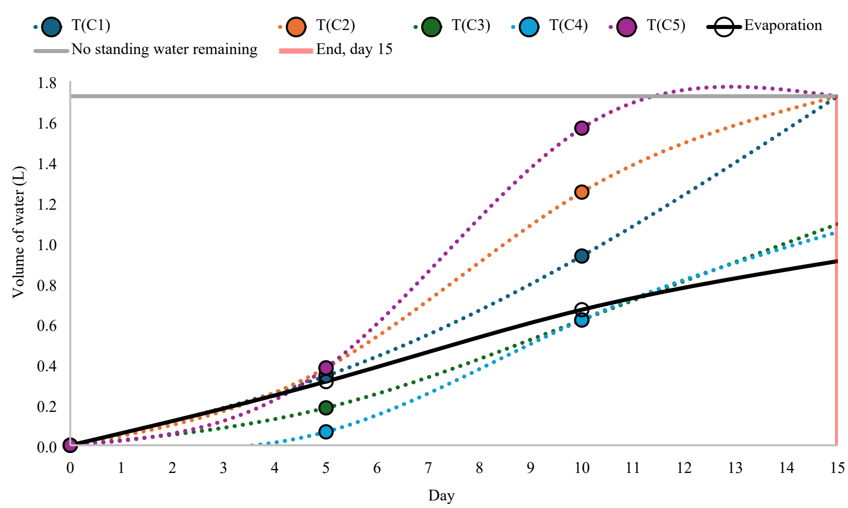

Figure S1: Transpiration of OSPW through cattails over time in plant reactors (n = 5).

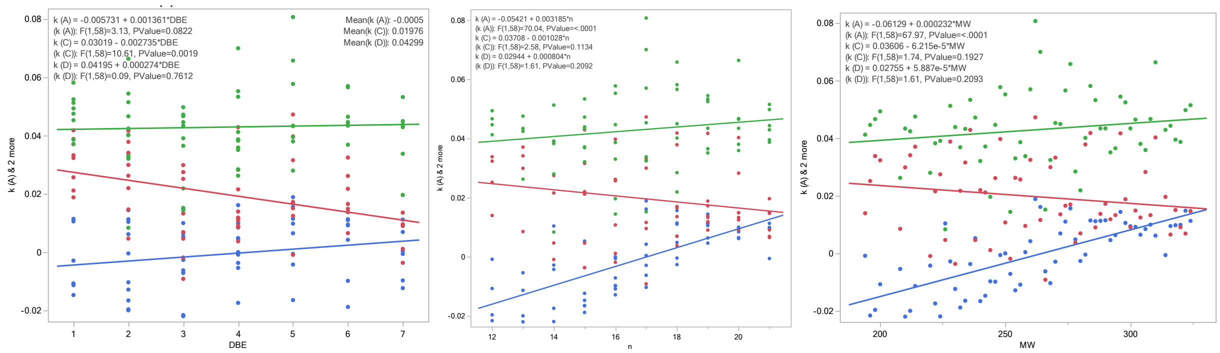

Figure S2: Linear regression of first-order depuration rate constants (kdep) as a function of double bond equivalents (DBE), carbon number (n), and molecular weight (MW, g/mol). Blue = OSPW only; Red = OSPW with peat soil; Green = cattail microcosm reactors.

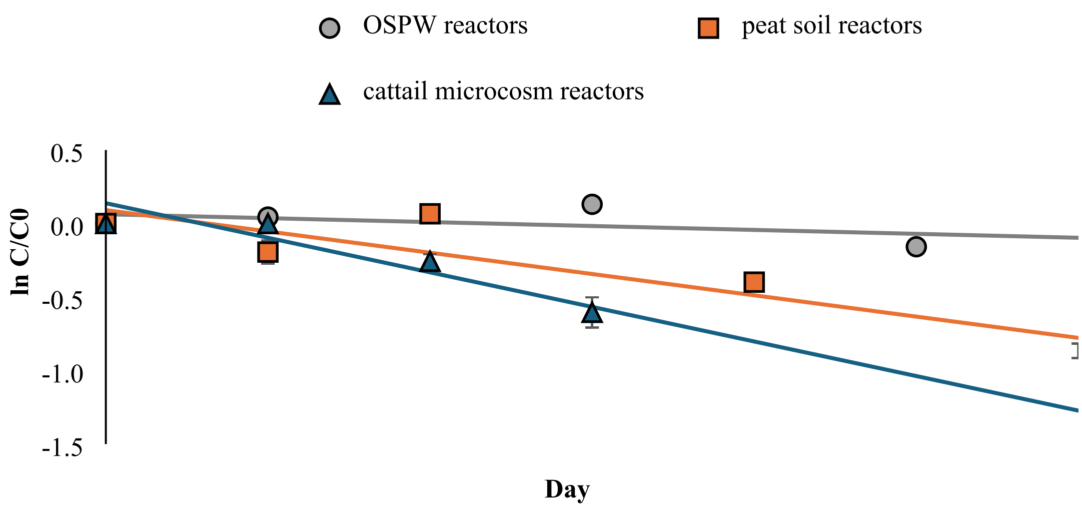

Figure S3: Normalized concentration of total (sum) O2-naphthenic acids in POCIS (C) to initial concentrations of total (sum) O2-naphthenic acids in POCIS on day 0 (C_0) from OSPW reactors, peat soil reactors, and cattail microcosm reactors over time. Error bars on data points represent standard error of the mean total (sum) of O2-naphthenic acids concentration.

Table S1: Weight of plant reactor components for all experimental units (group C) containing cattails.

rep	1	2	3	4	5
Weight of Soil + belowground biomass (g)	1513.4	1471.0	1979.5	1599.3	1593.2
Weight of aboveground biomass (g)	6.9	6.5	5.0	5.8	8.6
Weight of belowground biomass (g)	22.8	13.3	12.1	27.5	19.6
Weight of soil in reactor (g)	1490.6	1457.6	1967.4	1571.8	1573.6
Weight of above- and below-ground biomass (g)	29.7	19.8	17.1	33.3	28.2
Total weight of plant reactor (soil + above- + below-ground biomass) (g)	1520.3	1477.4	1984.5	1605.1	1601.8

Table S2: Rate of depuration (k_{dep}; day^{-1}) from OSPW in microcosm reactors with OSPW, OSPW and peat soil, and OSPW with cattail and peat soil by carbon number and double bond equivalent. Negative k_{dep} indicates the concentration of the O2-naphthenic acid was found to increase over time.

			OSPW reactors		**Peat soil reactors**		**Cattail microcosm reactors**	
n	**DBE**	**Chemical**	**k_{dep}**	**SE (k)**	**k_{dep}**	**SE (k)**	**k_{dep}**	**SE (k)**
12	1	C12H24O2	0.001	0.001	0.015	0.004	0.042	0.009
12	2	C12H22O2	0.003	0.003	0.032	0.006	0.049	0.011
12	3	C12H20O2	-0.005	0.004	0.034	0.007	0.047	0.013

12	4	C12H18O2	-0.009	0.003	0.025	0.007	0.045	0.011
13	1	C13H26O2	0.003	0.001	0.014	0.003	0.041	0.008
13	2	C13H24O2	0.006	0.004	0.037	0.007	0.048	0.013
13	3	C13H22O2	-0.003	0.004	0.034	0.008	0.042	0.014
13	4	C13H20O2	-0.008	0.004	0.030	0.007	0.043	0.014
14	1	C14H28O2	0.000	0.002	0.009	0.004	0.026	0.010
14	2	C14H26O2	0.014	0.004	0.039	0.008	0.051	0.016
14	3	C14H24O2	0.004	0.020	0.005	0.009	0.008	0.016
14	4	C14H22O2	-0.004	0.004	0.028	0.008	0.039	0.015
14	5	C14H20O2	-0.006	0.003	0.022	0.006	0.038	0.012
15	1	C15H30O2	-0.010	0.003	-0.001	0.005	0.028	0.006
15	2	C15H28O2	-0.002	0.003	0.021	0.006	0.037	0.014
15	3	C15H26O2	-0.003	0.004	0.022	0.006	0.032	0.015
15	4	C15H24O2	0.002	0.002	0.005	0.004	0.047	0.007
15	5	C15H22O2	0.017	0.005	0.043	0.010	0.053	0.020
15	6	C15H20O2	0.004	0.005	0.032	0.009	0.043	0.017
15	7	C15H18O2	-0.003	0.004	0.022	0.007	0.037	0.015
16	1	C16H32O2	-0.015	0.002	-0.004	0.007	0.044	0.013
16	2	C16H30O2	0.005	0.004	0.026	0.006	0.039	0.016
16	3	C16H28O2	0.003	0.004	0.026	0.006	0.033	0.016
16	4	C16H26O2	-0.014	0.003	-0.002	0.007	0.014	0.010
16	5	C16H24O2	0.001	0.001	0.011	0.004	0.055	0.008
16	6	C16H22O2	0.020	0.005	0.040	0.011	0.058	0.023
16	7	C16H20O2	0.007	0.004	0.026	0.008	0.045	0.018
17	1	C17H34O2	-0.009	0.002	0.001	0.006	0.020	0.007
17	2	C17H32O2	0.014	0.004	0.033	0.007	0.045	0.020
17	3	C17H30O2	0.008	0.004	0.030	0.007	0.032	0.018
17	4	C17H28O2	-0.010	0.002	-0.009	0.008	0.015	0.010
17	5	C17H26O2	0.012	0.002	0.012	0.006	0.070	0.010
17	6	C17H24O2	0.035	0.0045	0.047	0.014	0.081	0.028
17	7	C17H22O2	0.020	0.004	0.033	0.009	0.057	0.022
18	1	C18H36O2	0.001	0.002	0.010	0.004	0.034	0.006
18	2	C18H34O2	0.026	0.0036	0.042	0.009	0.058	0.023
18	3	C18H32O2	0.018	0.005	0.038	0.008	0.040	0.022
18	4	C18H30O2	-0.003	0.002	0.007	0.006	0.022	0.007
18	5	C18H28O2	0.001	0.002	0.004	0.012	0.028	0.010
18	6	C18H26O2	0.011	0.003	0.017	0.004	0.066	0.010
18	7	C18H24O2	0.008	0.003	0.017	0.004	0.057	0.009
19	1	C19H38O2	0.004	0.003	0.014	0.003	0.045	0.007

19	2	C19H36O2	0.007	0.003	0.019	0.004	0.053	0.009
19	3	C19H34O2	0.027	0.0036	0.042	0.009	0.055	0.025
19	4	C19H32O2	0.004	0.003	0.013	0.004	0.037	0.007
19	5	C19H30O2	0.002	0.003	0.012	0.005	0.035	0.007
19	6	C19H28O2	0.007	0.004	0.017	0.004	0.043	0.007
19	7	C19H26O2	0.007	0.004	0.014	0.004	0.043	0.007
20	2	C20H38O2	0.007	0.004	0.009	0.004	0.053	0.008
20	3	C20H36O2	0.020	0.005	0.040	0.010	0.066	0.020
20	4	C20H34O2	0.007	0.003	0.013	0.004	0.047	0.007
20	5	C20H32O2	0.005	0.003	0.028	0.004	0.036	0.009
20	6	C20H30O2	0.004	0.003	0.013	0.005	0.038	0.009
20	7	C20H28O2	0.005	0.004	0.015	0.004	0.047	0.007
21	2	C21H40O2	0.005	0.004	0.009	0.003	0.043	0.008
21	3	C21H38O2	0.007	0.004	0.015	0.003	0.052	0.008
21	4	C21H36O2	0.008	0.004	0.007	0.004	0.050	0.006
21	5	C21H34O2	0.009	0.003	0.009	0.004	0.039	0.008
21	6	C21H32O2	0.007	0.004	0.015	0.004	0.040	0.008
21	7	C21H30O2	0.005	0.004	0.007	0.004	0.044	0.008

Table S3: Summary of OSPW chemistry on day zero.

Parameter	units	OSPW (day 0)
Conductivity	uS/cm	1028
Turbidity	NTUs	3.7
Total Hardness as CaCO3	mg/L	250
Total Alkalinity as CaCO3	mg/L	250
Total Dissolved Solids	mg/L	900
Total Suspended Solids (TSS)	mg/L	4.9
Dissolved Inorganic Carbon (DIC)	mg/L	57
Dissolved Organic Carbon (DOC)	mg/L	22
Total Organic Carbon (TOC)	mg/L	21
Total O2-naphthenic acids*	mg/L	41

*Total O2-naphthenic acid concentrations in OSPW were measured by InnoTech Alberta (Edmonton, AB, Canada) and quantitation closely followed Pereira et al. (2013).

References:

Pereira, A. S., Bhattacharjee, S., & Martin, J. W. (2013). Characterization of Oil Sands Process-Affected Waters by Liquid Chromatography Orbitrap Mass Spectrometry. *Environmental Science & Technology*, *47*(10), 5504–5513. https://doi.org/10.1021/es401335t