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Supporting Information for

Modeling Comprehensive Chemical Composition of Weathered Oil Following a Marine Spill to Predict Transport, Ozone and Potential Secondary Aerosol Formation and Constrain Transport Pathways

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Introduction

- This supporting information covers the updated yields for potential secondary aerosol from hydrocarbon precursors, specifically for oxidation conditions of low-NOx levels. These yields are updated to reflect current laboratory experiments. The time-resolved, speciated yields for PSOA are also shown, as an indicator of which emissions would lead to SOA at a given point during evaporation of DWH oil.

Table S1. Fractional potential secondary organic aerosol yields for C1-C25 hydrocarbons for 8 classes of hydrocarbons (n-alkanes, branched-alkanes, cyclic alkanes (cyc1), branched-cyclic alkanes (cyc1-2), bi-cyclic alkanes (cyc2), tricyclic alkanes (cyc3), alkyl-benzenes (arom), and polycyclic aromatic hydrocarbons (PAH).

	nALk	brAlk	cyc1	cyc1-2	cyc2	cyc3	Arom	PAH
1	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0
6	0	0	0.004	0.004	0	0	0.1	0.1
7	0	0	0.01	0.007	0	0	0.12	0.12
8	0.0036	0.0042	0.06	0.015	0	0	0.14	0.14
9	0.0072	0.0084	0.09	0.031	0.005	0	0.15	0.15
10	0.0156	0.0182	0.095	0.059	0.01	0	0.16	0.17
11	0.0318	0.0371	0.12	0.1	0.018	0	0.17	0.23
12	0.06	0.07	0.16	0.16	0.031	0.032	0.19	0.28
13	0.14	0.133	0.26	0.26	0.056	0.057	0.26	0.4
14	0.22	0.231	0.41	0.41	0.097	0.098	0.33	0.49
15	0.31	0.385	0.58	0.64	0.16	0.17	0.39	0.62
16	0.4	0.534	0.65	0.8	0.26	0.27	0.43	0.7
17	0.49	0.6	0.73	0.8	0.44	0.45	0.46	0.75
18	0.58	0.63	0.81	0.8	0.6	0.73	0.51	0.79
19	0.67	0.67	0.86	0.8	0.7	0.8	0.56	0.82
20	0.76	0.7	0.92	0.8	0.8	0.8	0.61	0.82
21	0.845	0.72	0.97	0.8	0.85	0.8	0.65	0.82
22	0.925	0.73	1.03	0.8	0.9	0.8	0.67	0.82
23	0.995	0.74	1.04	0.8	0.94	0.8	0.68	0.82
24	1.055	0.75	1.06	0.8	0.96	0.8	0.68	0.82
25	1.095	0.75	1.09	0.8	0.98	0.74	0.68	0.82

Figure S1. Speciated PSAO "fluxes" during the evaporation of DWH oil for the deep-sea case (reduction by 50% of >C10 aromatics) for a slick with 0.15mm thickness. These results directly correspond to the left panel of Figure 9. Colors correspond to hydrocarbon classes: n-alkanes (red), branched linear alkanes (magenta), monocyclic alkanes (orange), branched monocyclic alkanes (purple), bi- and tri-cyclic alkanes (green), polycyclic aromatics and alkyl benzene compounds (black). The yields correspond to the end-point yields of

SOA from the real-time evaporative emissions. The inset shows the high fluxes within 15 minutes of evaporation, aromatics dominate at very short times.