Supplementary Information

Air Quality Predictions using Measurement-Derived Organic Gaseous and Particle Emissions in a Petrochemical-Dominated Region

Craig A Stroud[1], Paul A Makar[1], Junhua Zhang[1], Michael D. Moran[1], Ayodeji Akingunola[1], Shao-Meng Li[1], Amy Leithead[1], Katherine Hayden[1], and May Siu[2]

[1]Air Quality Research Division, Environment and Climate Change Canada, 4905 Dufferin Street, Toronto, Ontario, M3H 5T4, Canada

[2]Air Quality Research Division, Environment and Climate Change Canada, 335 River Road, Ottawa, Ontario, K1V 1C7, Canada

Corresponding author: Craig A. Stroud (craig.stroud@canada.ca)

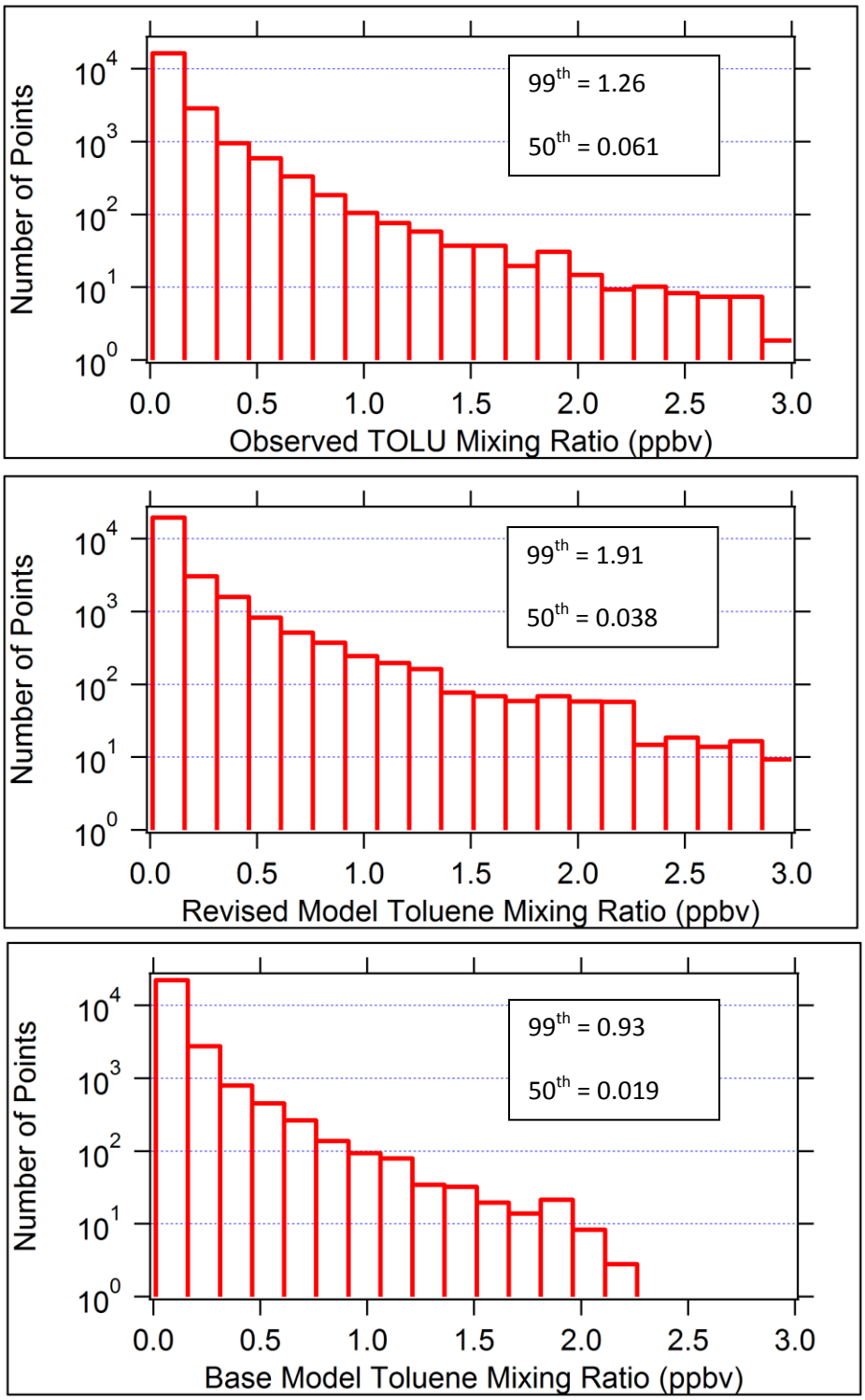
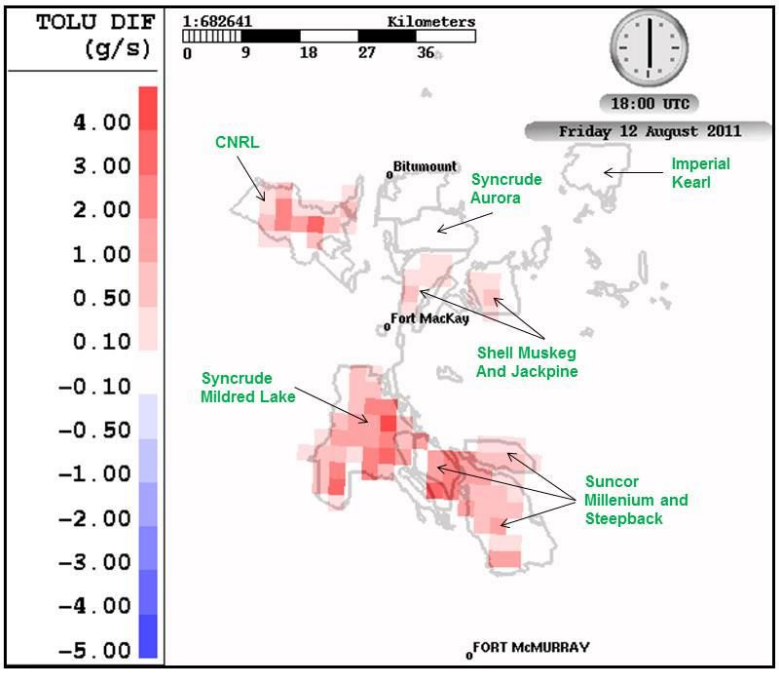


Figure S1. Histograms for (a) observed TOLU, (b) revised-emissions TOLU, and (c) base-case-emissions TOLU volume mixing ratios (ppbv). Points correspond to 10-sec averaged aircraft and model data, sorted into 20 bins by volume mixing ratio. The inset boxes show the 50th and 99th percentile values for each histogram.



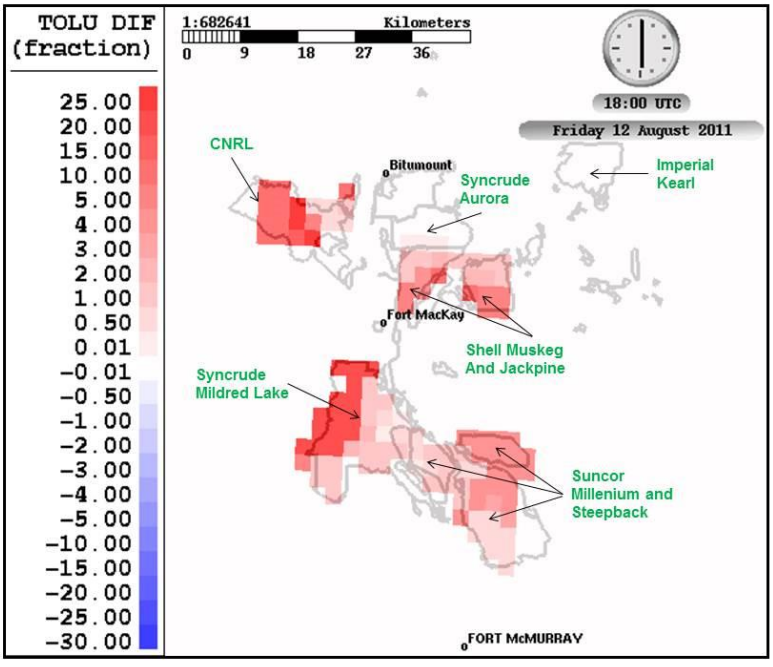


Figure S2. (a) Difference in lumped TOLU emissions (revised-base case) in units of grams/sec for each 2.5-km x 2.5-km grid cell; (b) relative difference calculated as (revised–base)/base.

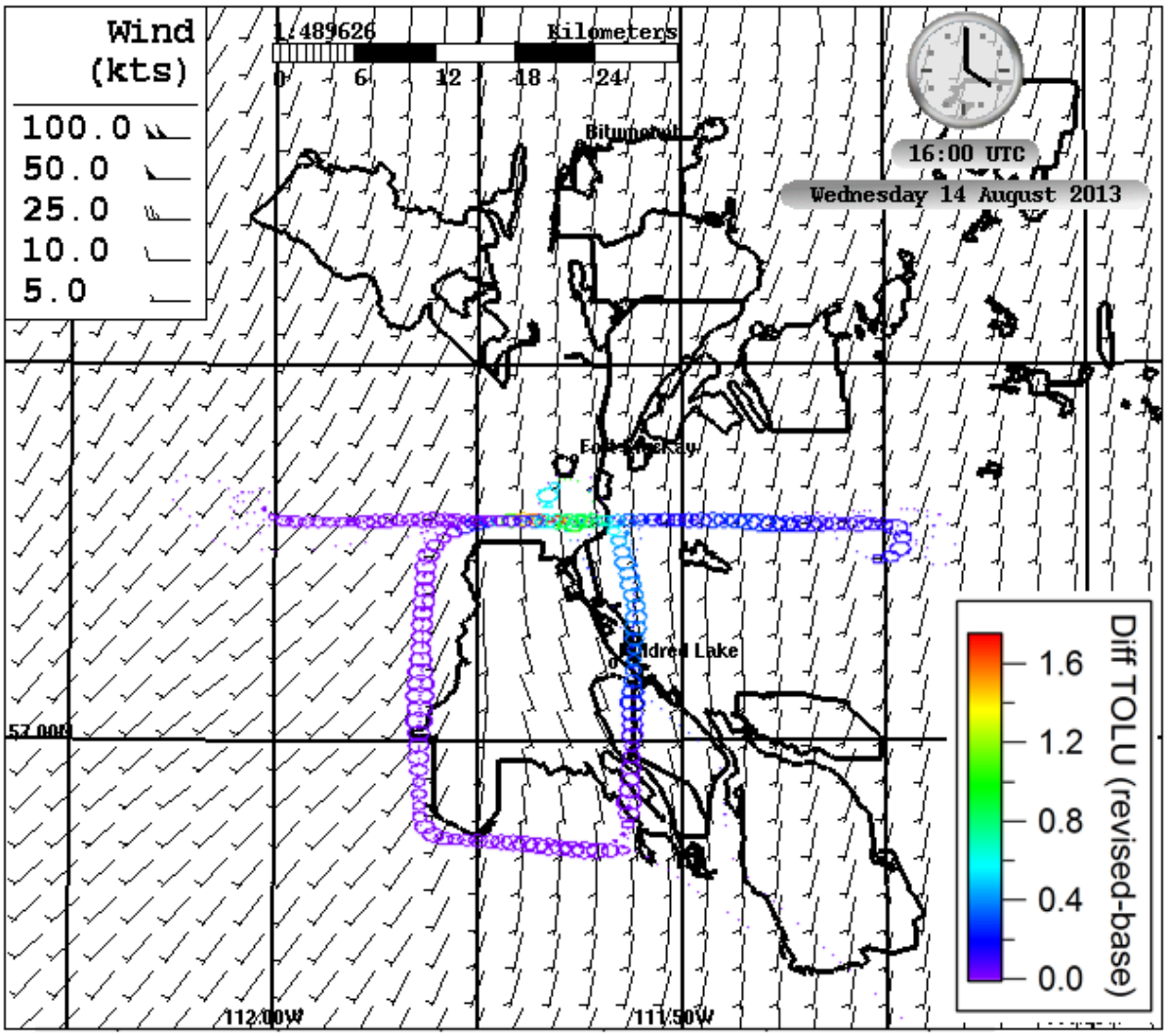


Figure S3. Flight track of the aircraft on Aug. 14, 2013 around the Syncrude Mildred Lake facility color-coded by the difference in TOLU volume mixing ratio (pptv) between the revised-emissions and the base-case simulations. The modelled wind barbs at the time of the maximum difference (16 UTC) are included in the background map.

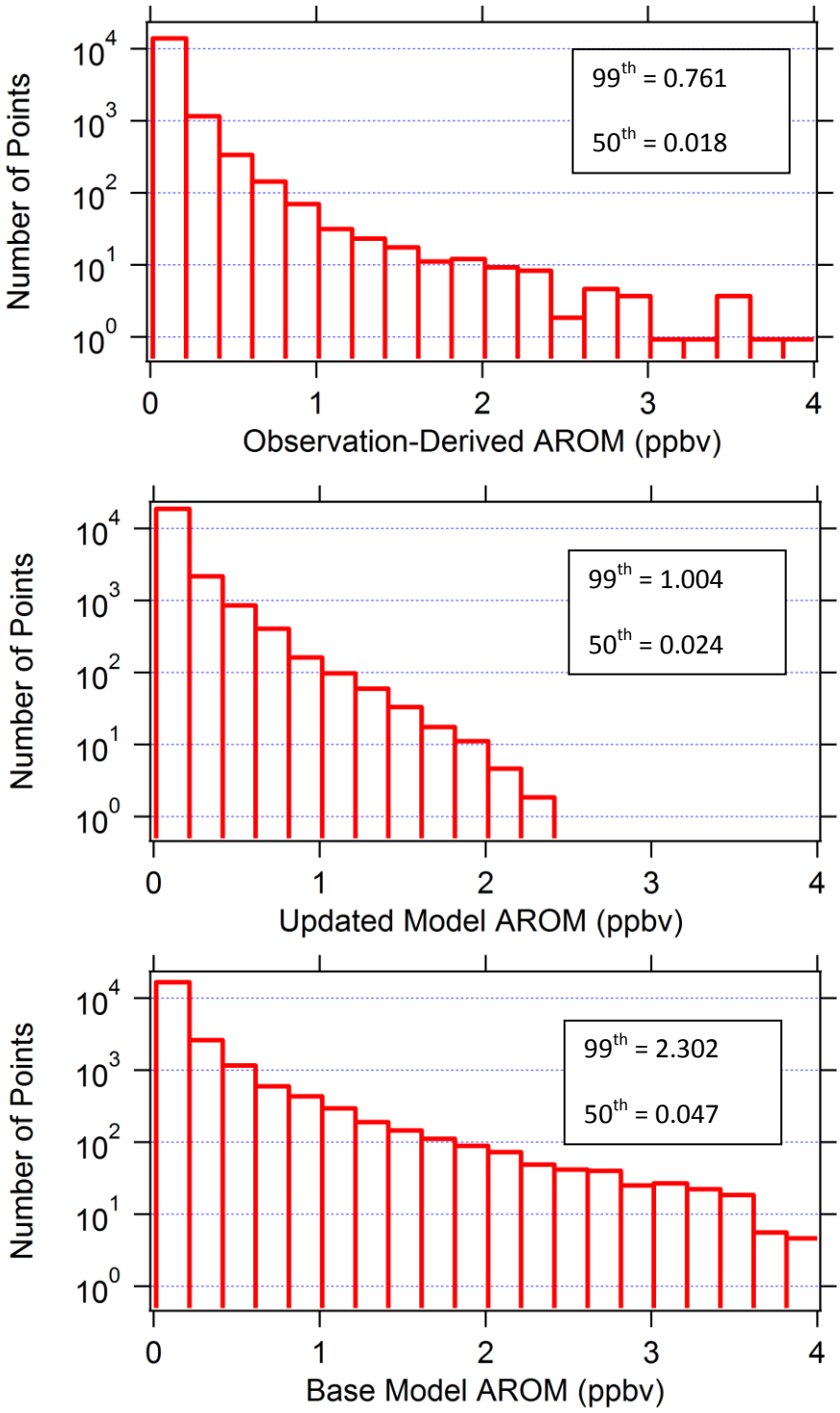
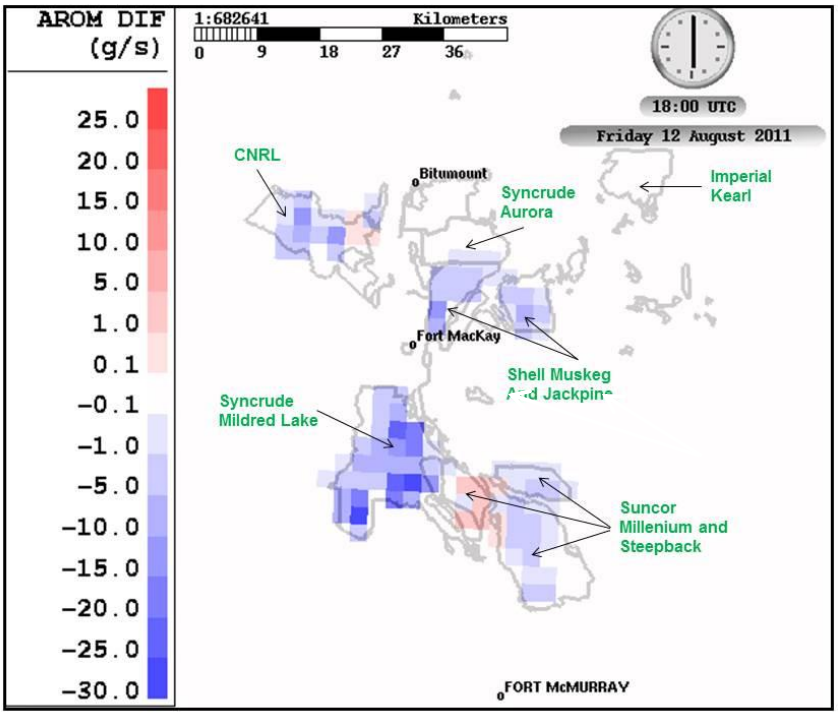


Figure S4. Histograms for (a) observed AROM, (b) revised-emissions AROM, and (c) base model AROM volume mixing ratios (ppbv). Points correspond to 10-sec averaged aircraft and model data, sorted into 20 bins by volume mixing ratio. The inset boxes show the 50th and 99th percentile values for each histogram.



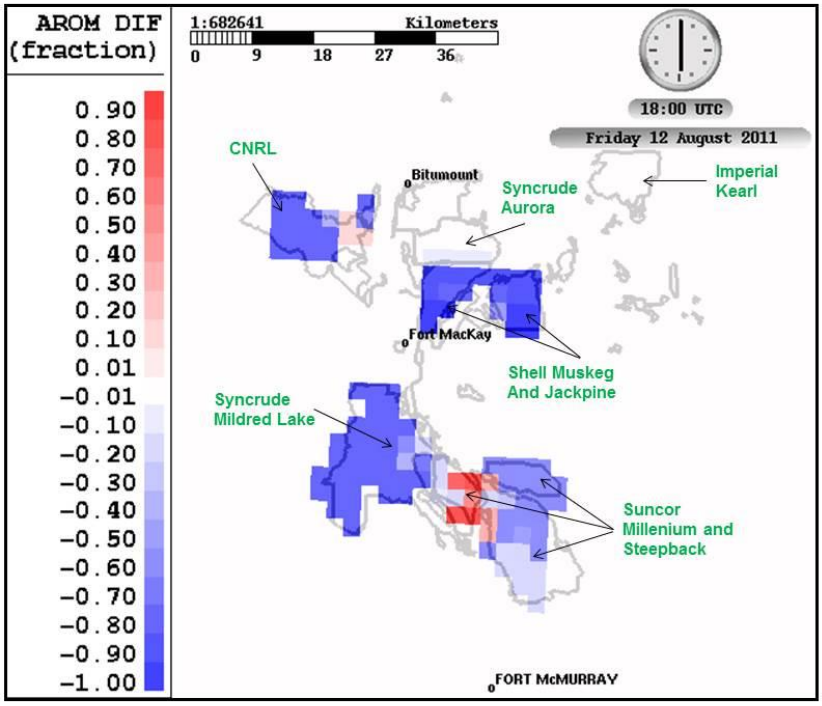


Figure S5. (a) Difference in AROM emissions (revised-base case) in units of grams/sec for a selected date and time; (b) relative difference calculated as (revised–base)/base. Large negative changes are noted over the Syncrude Mildred Lake facility.

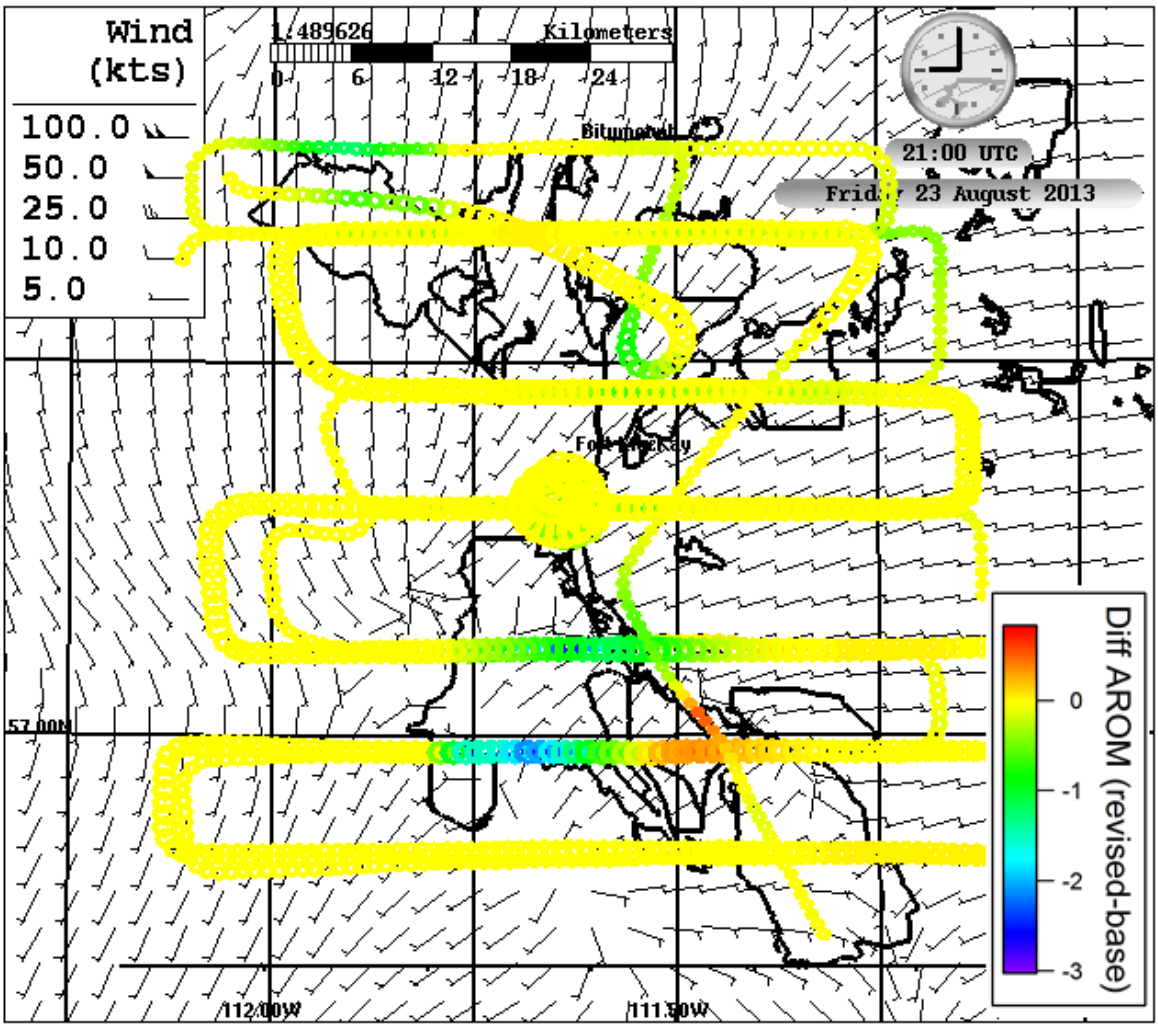


Figure S6. Flight track of the aircraft on Aug. 23, 2013 over all six OS surface mines color-coded by the difference in predicted AROM volume mixing ratio (pptv) between the revised-emissions and the base-case simulations. The modelled wind barbs at the time of the maximum difference (21 UTC) are included in the background map.

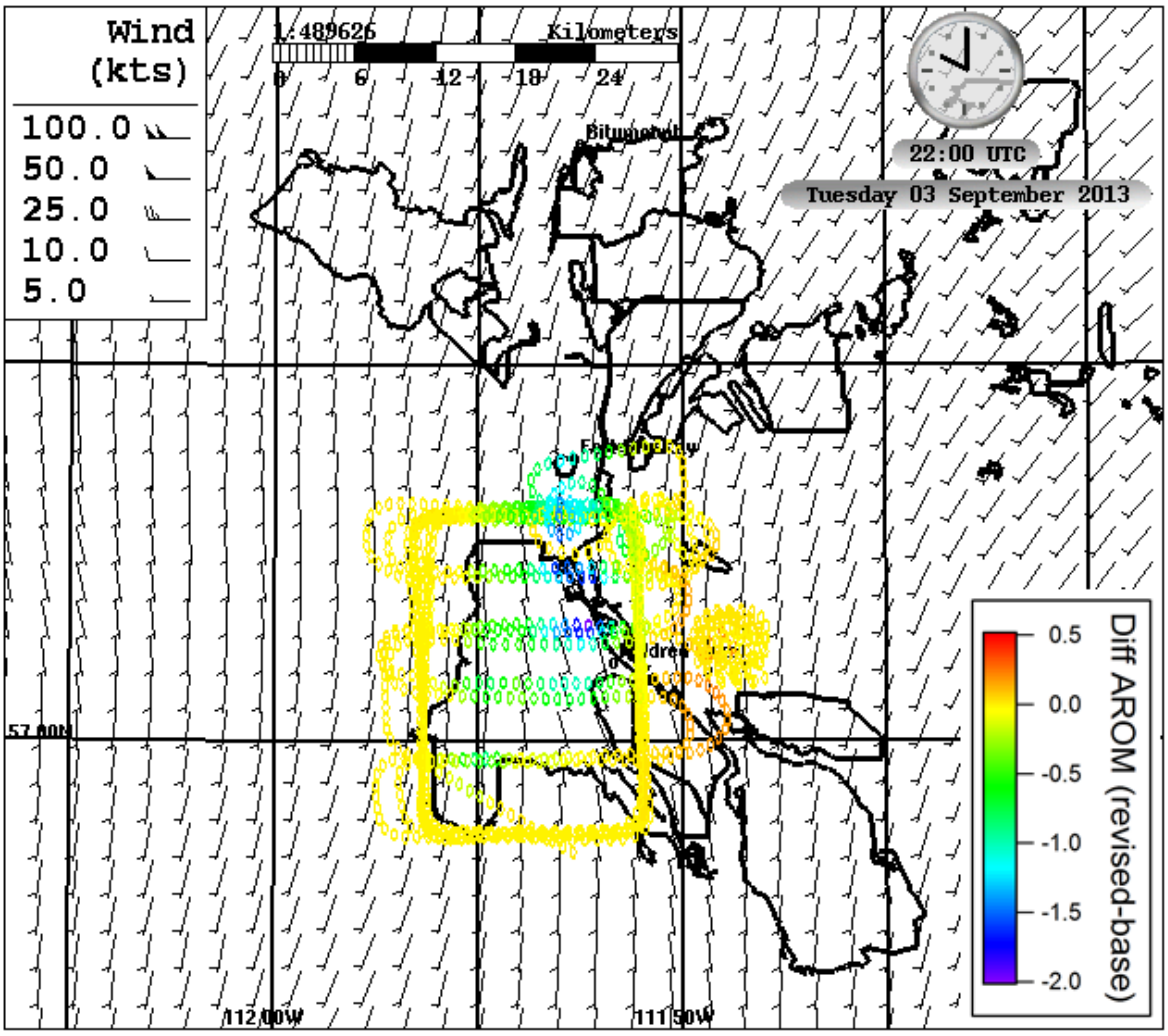


Figure S7. Flight track of the aircraft on Sept. 3, 2013 over the Syncrude Mildred Lake facility color-coded by the difference in predicted AROM volume mixing ratio (pptv) between the revised-emissions and the base-case simulations. The modelled wind barbs at the time of the maximum difference (22 UTC) are included in the background map.

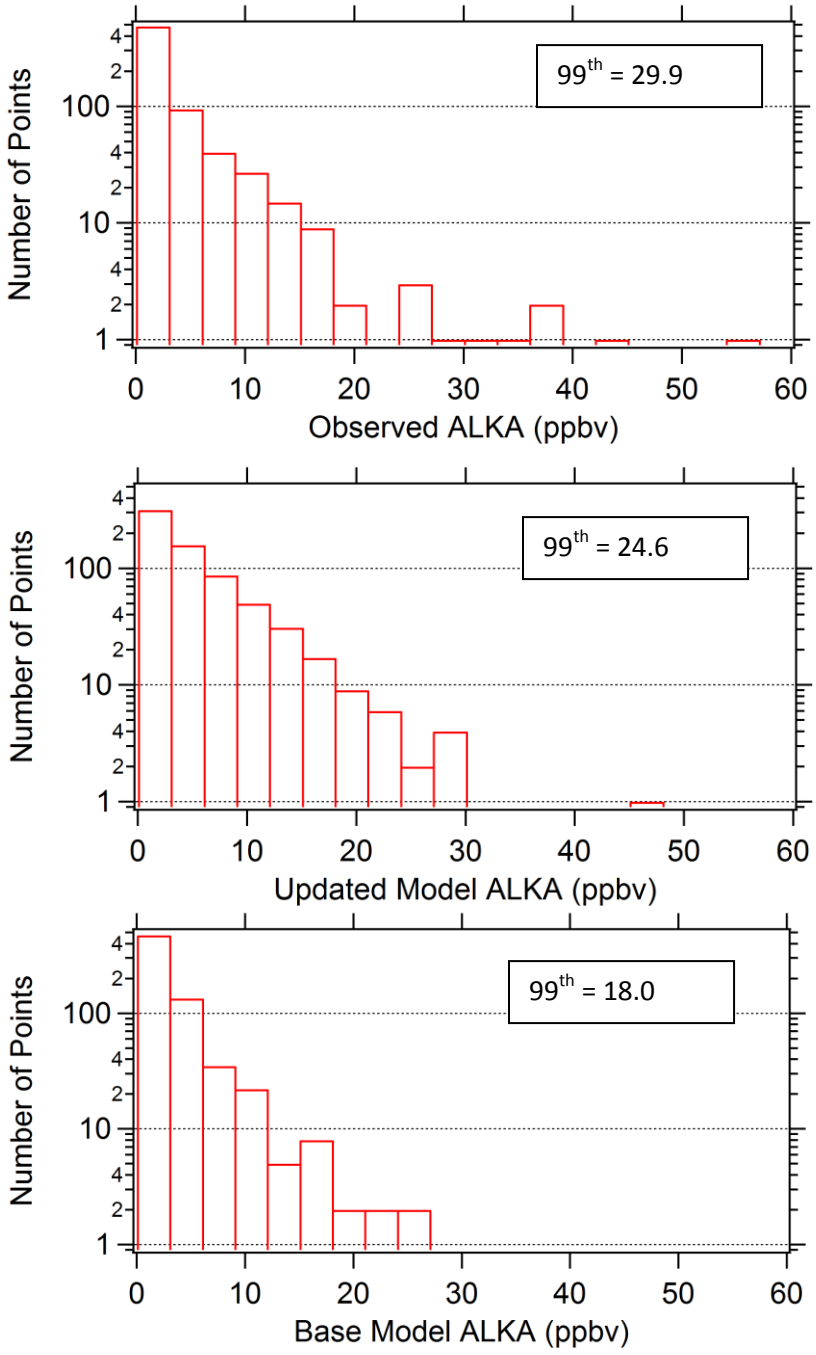
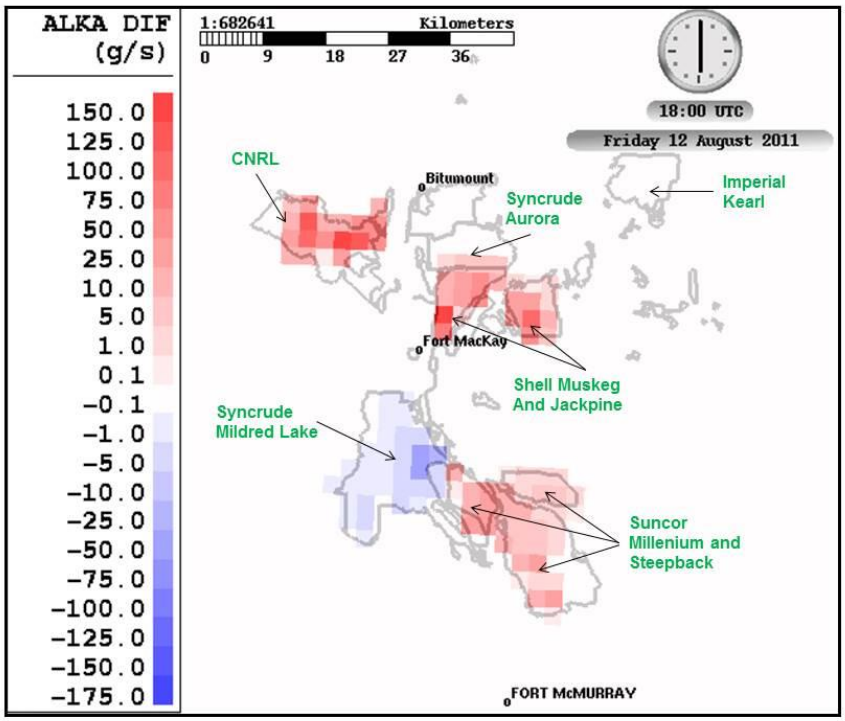


Figure S8. Histograms for (a) observed ALKA, (b) revised-emissions ALKA, and (c) base-case emissions ALKA volume mixing ratios (ppbv). Points correspond to canister grab samples and model data, sorted into 20 bins by mixing ratio. The inset boxes show the 99th percentile value for each histogram.



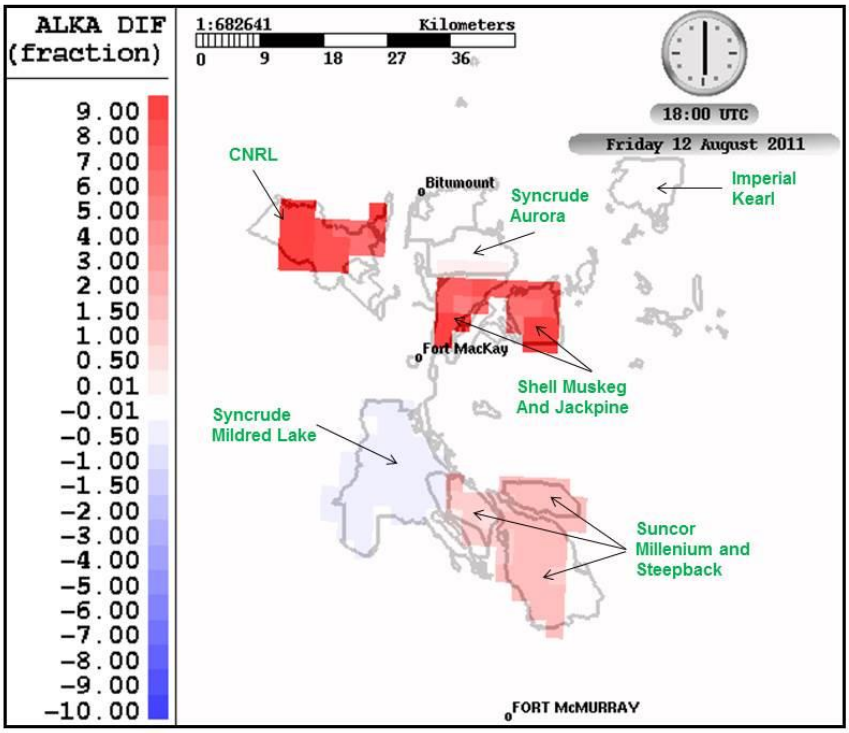


Figure S9. (a) Difference in lumped ALKA emissions (revised-base case) in units of grams/sec for each 2.5-km x 2.5-km grid cell; (b) relative difference calculated as (revised–base)/base.

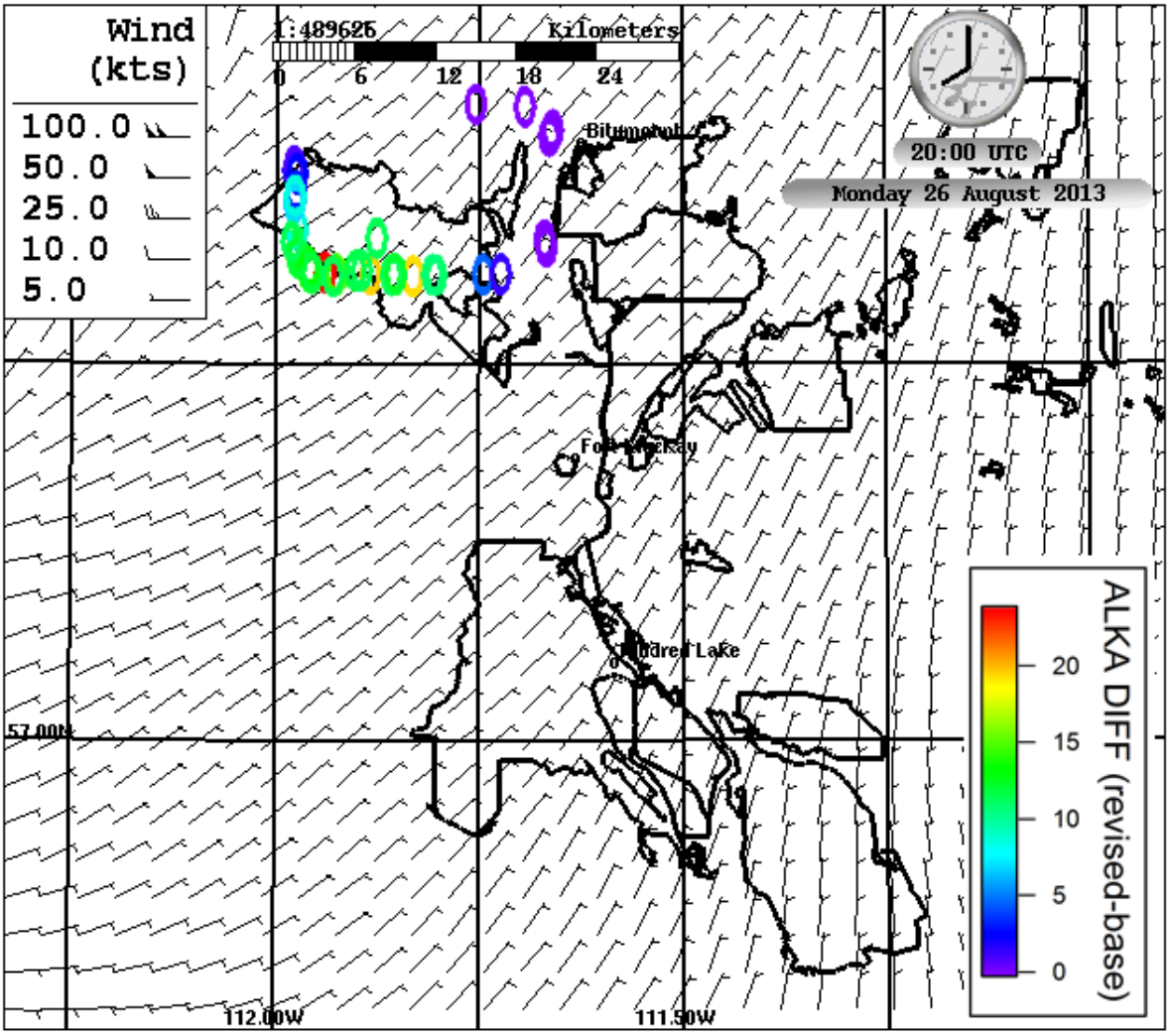


Figure S10. Flight track of the aircraft on Aug. 26, 2013 over the CNRL Horizon facility color-coded by the difference in predicted ALKA volume mixing ratio (pptv) between the revised-emissions and the base-case simulations. The modelled wind barbs at the time of the maximum difference (20 UTC) are included in the background map.

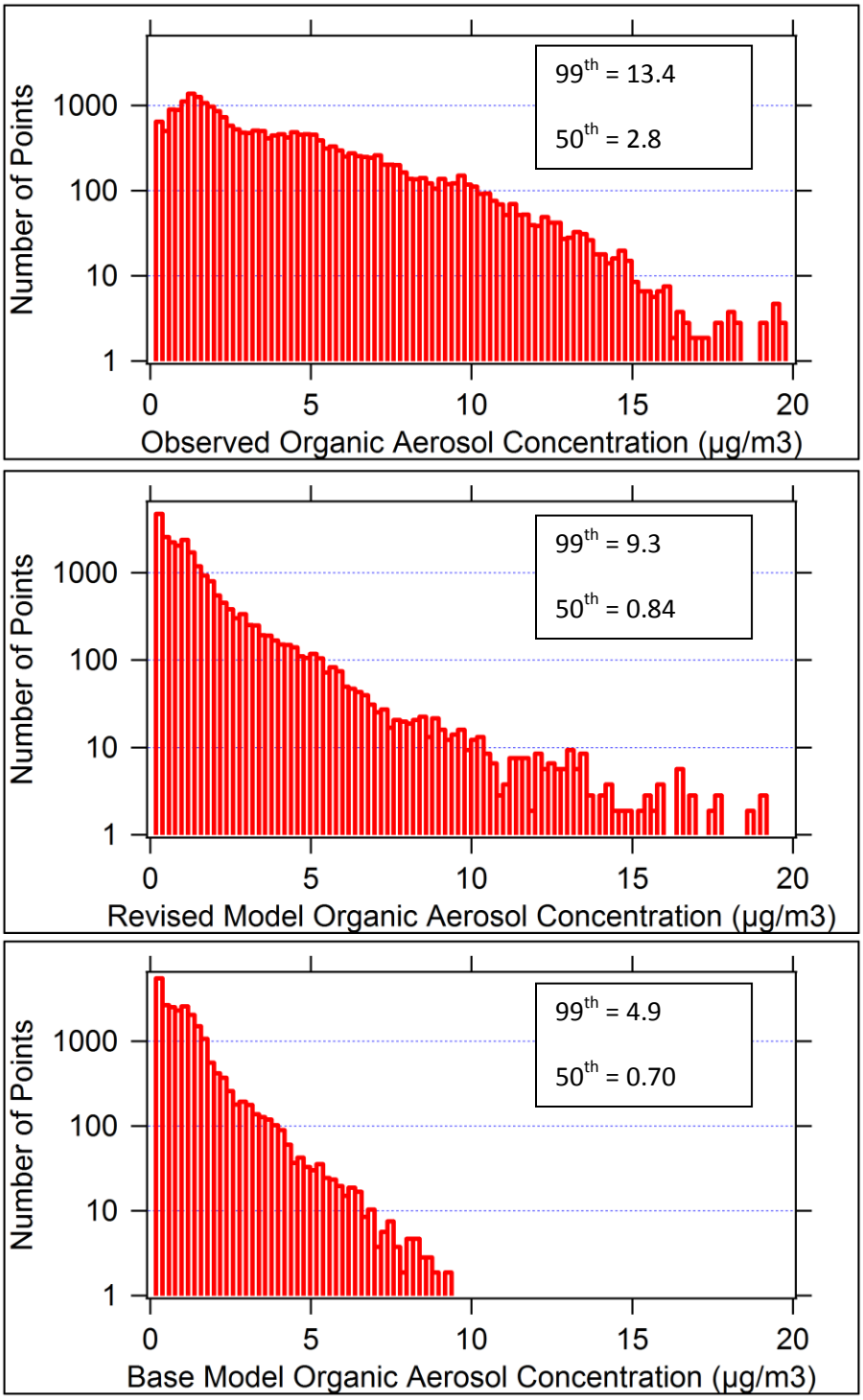
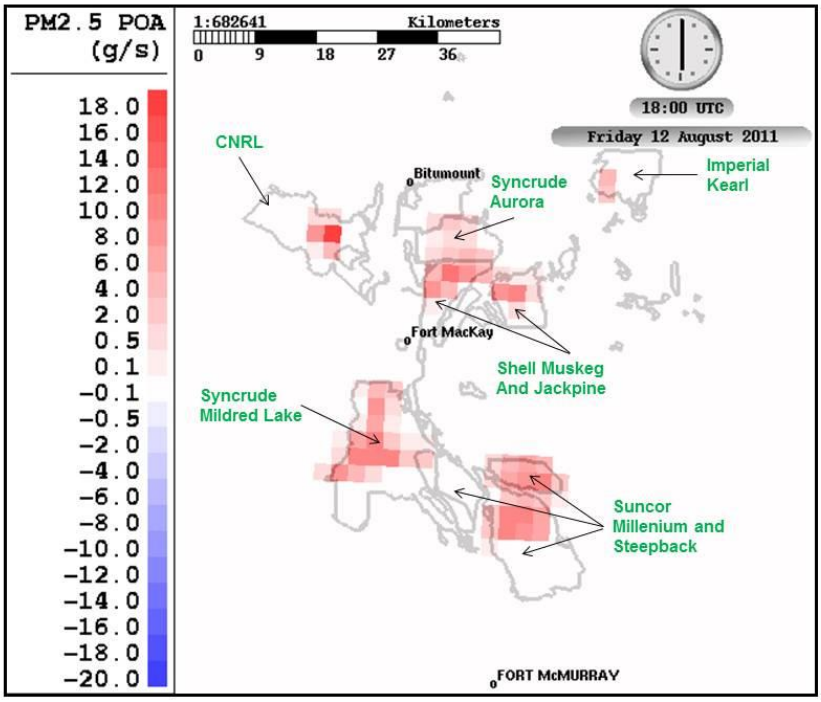


Figure S11. Histograms for (a) observed organic aerosol (OA), (b) revised-emissions OA, and (c) base-case emissions OA concentrations (µg/m^3). Points correspond to 10-sec averaged aircraft and model data. The inset boxes show the 50th and 99th percentile values for each histogram.



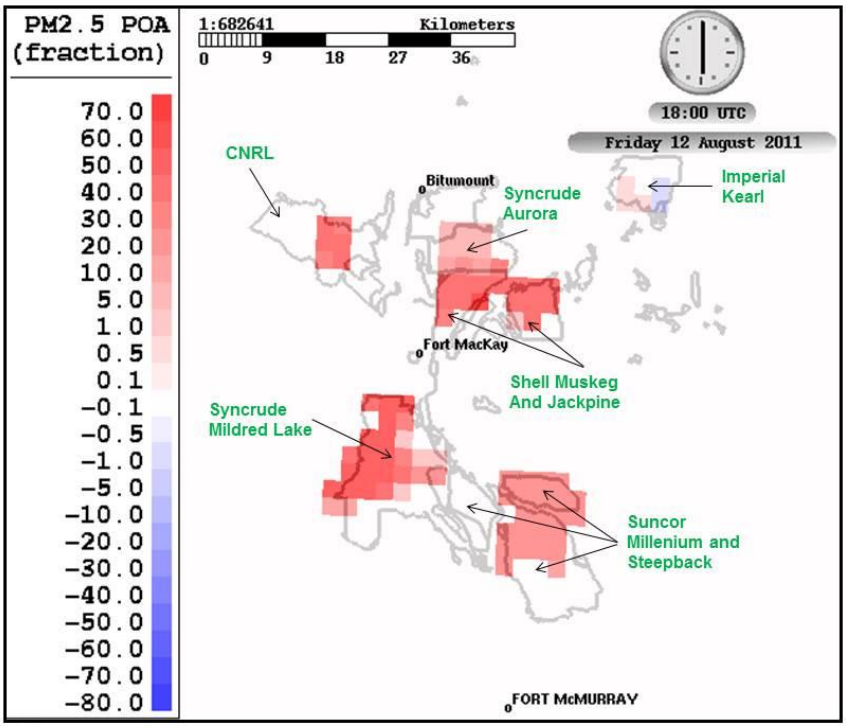


Figure S12. (a) Difference in primary organic aerosol (POA) emissions (revised-base case) in units of grams/sec for each 2.5-km x 2.5-km grid cell; (b) relative difference calculated as (revised–base)/base.

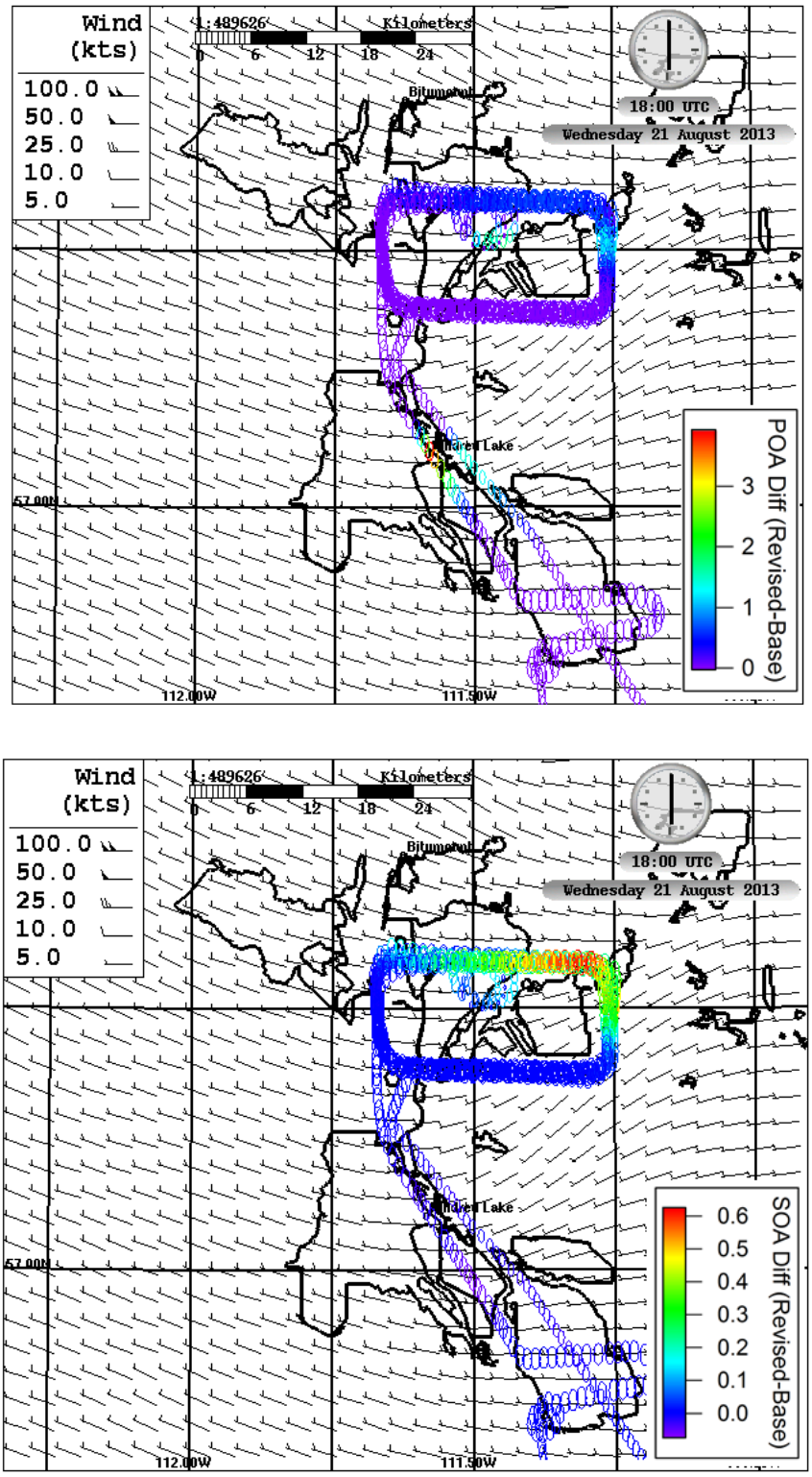


Figure S13. Flight track of the aircraft on Aug. 21, 2013 over the Shell Muskeg/Jackpine facility color-coded by the difference in predicted (a) POA concentration (μg/m^3) and (b) SOA concentration between the revised-emissions and the base-case-emissions simulations.

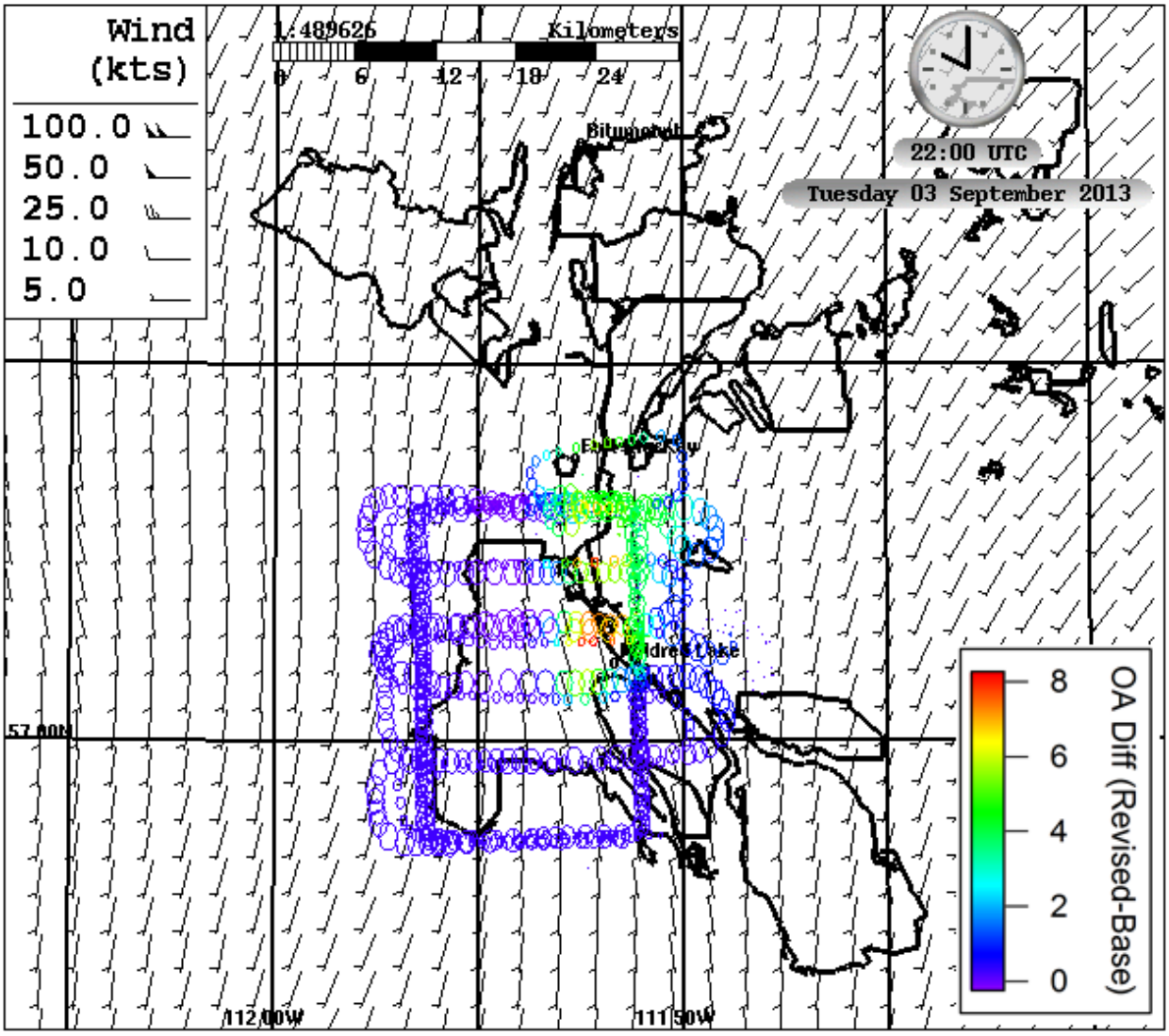


Figure S14. Flight track of the aircraft on Sept. 3, 2013 over the Syncrude Mildred Lake facility color-coded by the difference in predicted organic aerosol (OA) concentration (μg/m^3) between the revised-emissions and the base-case-emissions simulations.

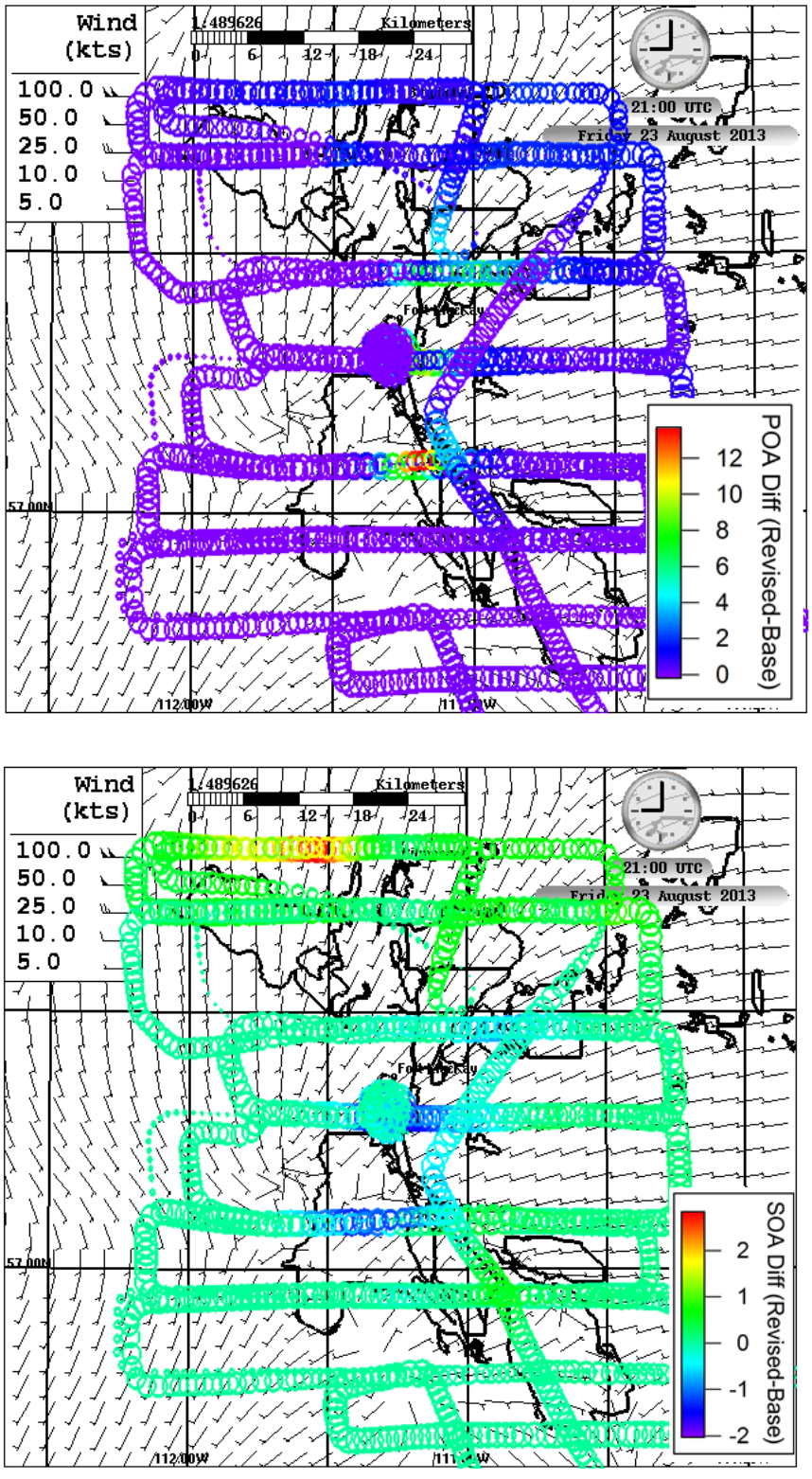


Figure S15. Flight track of the aircraft on Aug. 23, 2013 over all six OS surface mines color-coded by the difference in predicted (a) POA concentration (µg/m^3) and (b) SOA concentration between the revised-emissions and the base-case-emissions simulations.

Table S1. Composite VOC speciation profiles (mass fractions) applied to the surface mining facilities in the Athabasca oil sands region compared to speciation profiles for petrochemical refineries in the U.S. Houston area (in ADOM-II chemical speciation). Data are based on Zhang *et al.* (2017) and references therein.

Species	Shell M/J, Suncor AN, Imperial Kearl	Syncrude ML, Suncor, CNRL	Base case CEMS profile #9012	Base case SPECIATE profile #0316
EC38 (Propane, Benzene, Acetylene)	0.0	0.0	0.247	0.176
EA3 (Alkane ≥C4)	0.90	0.71	0.623	0.781
EA2 (Alkene ≥C3)	0.007	0.069	0.031	0.002
ETOL (Toluene and other mono-aromatics)	0.001	0.057	0.005	0.008
EARO (Multi-functional aromatics)	0.0003	0.099	0.003	0.003
EHCO (Formaldehyde)	0.00001	0.0003	0.110	0.0

Columns do not add up to unity due to unaccounted for or unassigned species or due to consideration of reactivity weighting for the ADOM-II mechanism.

Base case profile #9012 is a profile from the Canadian Emissions Processing System (Moran, M.D., M.T. Scholtz, C.F. Slama, A. Dorkalam, A. Taylor, N.S. Ting, D. Davies, P.A. Makar, S. Venkatesh, An Overview of CEPS1.0: Version 1.0 of the Canadian Emissions Processing System for Regional-Scale Air Quality Models. In Proc. 7th AWMA Emission Inventory Symp., Research Triangle Park, North Carolina, Air & Waste Management Association, Pittsburgh, Oct. 28-30, 1997.)