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Emissions preparation and analysis for multiscale air quality modeling over the Athabasca Oil Sands Region of Alberta, Canada

Junhua Zhang et al.

Correspondence to: Junhua Zhang (junhua.zhang@canada.ca)

Supplement Material:

S1. Phase 1 hybrid emissions inventory and ancillary files

Prior to the 2013 AOSR field study, the 10 inventories listed in Table S1 by name, target region, and base year were reviewed to choose the most suitable emissions inventory data for AQ modelling for the OS area (AESRD, 2013; Marson, 2013). After an intensive review of these newer inventories, it became clear that no one inventory was the "best" choice in all respects, but three inventories contained emissions data that were either unique (i.e., not reported elsewhere), more detailed, and/or the most recent. The 2009-2010 Cumulative Environmental Management Association (CEMA) inventory (Davies et al., 2012) had the most detailed stack- and process-level emissions for the AOSR surface mining facilities shown in Figure 1 (including separate emissions from mine faces, tailings ponds, and off-road mine hauler fleets, except for fugitive dust emissions from the off-road fleet); the 2010 Canadian NPRI included emissions for some species (NH_3 and PM_{10}) and source types (fugitive dust emissions from OS mine fleets) missing from the CEMA inventory; and the 2010 Canadian APEI from ECCC was the most comprehensive and had the largest spatial coverage (national) for area sources. Note, however, that at this time the 2010 Canadian APEI was not yet available in the detailed format required for emissions processing (referred to as the AQ modelling version), which requires the published APEI data to be transferred to a format that is suitable for processing emissions for AQ modelling as well as the addition of more detailed emissions data, such as monthly on-road and off-road emissions and process-based separation of emissions from some sectors (e.g., evaporative vs. exhaust emissions from on-road vehicles).

The solution adopted in the first phase for the best base-case inventory to use to generate GEM-MACH emissions input files for the 2013 field study was to create a synthesized or hybrid AQ modelling emissions inventory, as summarized in Table S2, that combined the best available information from the above inventories. The 2009-2010 CEMA inventory, supplemented by the 2010 NPRI for NH_3 and PM_{10} emissions, was mainly used to provide emissions for the AOSR field-study area while the 2006 APEI was used outside the AOSR where the CEMA inventory's coverage ended. The 2010 NPRI was also used to scale the CEMA facility-total VOC emissions for the five AOSR surface mines active at that time (Figure 1), since it was found that the CEMA inventory had the lowest total VOC emissions for these five facilities compared to four other inventories (ECCC & AEP, 2016) and the NPRI is Canada's legislated inventory of large point sources based on emissions reported by facilities. The ratio of 2010 NPRI total VOC emissions for the five mining facilities vs. the CEMA total yielded a scaling factor of 2.6, which was applied to the CEMA facility-total VOC emissions for the individual facilities (Table 1), as large uncertainties may exist in both inventories and the use of a uniform scaling factor should not affect the impact of VOC emissions from the OS facilities as a whole. One reason to focus on the VOC emissions from these five facilities was that for 2010 they were estimated by NPRI to have contributed 75% of VOC emissions from all Alberta facilities. The 2009-2010 CEMA inventory was also used to specify the process-specific allocation of these facility-total

emissions between mine faces, tailing ponds, plants, and smoke stacks, which then dictated the spatial and temporal allocation and chemical speciation of these process-level emissions (ECCC & AEP, 2016).

The focus of the OS field study was a roughly 100 km by 100 km subregion of the AOSR located north of Fort McMurray, Alberta (Figure 1). This study area contains a complex of six large surface bitumen mining and processing facilities situated on both sides of the Athabasca River. As shown in Figure 1, each mining facility covers a very large area, ranging from 66 to 275 km^2, and each facility contains various area sources within their boundaries, including NOx, CO, VOC, and $PM_{2.5}$ emissions from each mine's off-road heavy-hauler fleet, evaporative VOC emissions from tailings ponds and mine faces, and point sources of SO_2, NO_x, CO, VOC, $PM_{2.5}$ and fugitive VOC emissions from extraction and upgrading plants (Zhang et al., 2015). Although emissions from industrial facilities are normally treated as point sources by emissions processing systems and AQ models (e.g., Houyoux et al., 2000), each of these six facilities spans more than 10 GEM-MACH 2.5-km grid cells (area of 6.25 km^2 each), and many of the emissions are distributed over large areas within the facility boundaries. Treating such large facilities as point sources that can be assigned to a single grid cell is thus not realistic.

To address this concern, a new approach was taken in which these nominal point sources were treated as area sources. First, a GIS shapefile based on data collected by AESRD was obtained for the year 2010 with detailed locations of mine faces, extraction plants (and, for three facilities, upgrading plants), and tailings ponds for the five AOSR mines that were active within the study area at that time: Suncor Millenium and Steepbank mines; Syncrude Mildred Lake mine; Syncrude Aurora North mine; Shell Canada Muskeg River mine and Jackpine mine (known collectively as the Shell Canada Albian Sands mine); and CNRL Horizon mine (Figure 1). This shapefile was then used to develop three spatial surrogates for each facility to be used for spatial allocation of mine-face, extraction/upgrading plant, and tailings-pond emissions, respectively, including emissions from the off-road mining fleet and evaporative VOC emissions from mine faces, extraction plants, and tailing ponds (Zhang et al., 2015). It was assumed that the off-road fleets operated mainly in the mine-face areas, so the mine-face spatial surrogate field was used to allocate CAC emissions from the off-road fleet as well as evaporative VOC emissions from the mine faces. Note that emissions from the main smokestacks of the facilities were still treated as point sources. Finally, once all of the above development work was completed, the hybrid phase 1 emissions inventory was input to the SMOKE (Sparse Matrix Operator Kernel Emissions) emissions processing system (https://www.cmascenter.org/smoke) together with the new AOSR facility-specific spatial surrogate fields to generate phase 1 model-ready emissions input files for use by GEM-MACH during the 2013 summer field study (Zhang et al., 2015).

S2. Phase 2 hybrid emissions inventory and ancillary files

In phase 2, after the field study, emissions updates were made during the 2014-2015 period to include newly available emissions information, including (i) an AQ modelling version of the 2010 Canadian APEI, (ii) a preliminary version of the 2013 NPRI point-source inventory, (iii) stack-level continuous emission monitoring system (CEMS) measurements for 17

smokestacks at four AOSR mining facilities for the field-study months of August and September 2013, and (iv) daily reports of SO_2 emissions during abnormal operating conditions from one AOSR mining facility (CNRL Horizon) during a one-week period in August 2013 when up to 20 times normal daily SO_2 emissions were released to the air during several upset events (ECCC & AEP, 2016). The six inventories and other emissions data sources that were used to create a second hybrid Canadian AQ modelling emissions inventory for 2013 are listed in Table S3.

The GIS shapefile describing the OS mines was also updated using 2013 satellite imagery (Zhang et al., 2015). These shapefile updates captured growth in the boundaries of existing mine faces and tailings ponds as well as new mine faces and tailings ponds that had been opened post-2010, and they were used to update the facility-specific spatial surrogate fields. In addition, a sixth mine, the Imperial Oil Kearl mine, had entered production in 2013 (see Figure 1). Annual emissions estimates for this facility were obtained from the preliminary 2013 NPRI and three new spatial surrogates were developed to allocate emissions from this facility (Zhang et al., 2015). As well, monthly facility-specific bitumen production data reported to the province of Alberta for 2013 for the six OS mining facilities were used to create facility-specific monthly temporal profiles (Alberta Energy Regulator (AER), 2014; Zhang et al., 2015). Note that a more comprehensive and detailed description of the phase 2 hybrid inventory, the updated ancillary data sets for emissions processing, and the emissions processing procedure that was followed with the SMOKE system to generate model-ready emissions input files using the phase 2 inventory is available in the JOSM report (ECCC & AEP, 2016).

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Table S1: Emissions inventories reviewed in phase 1 prior to the 2013 AOSR field study.

Inventory Name	Geographic Coverage	Base Year
Cumulative Environmental Management Association (CEMA) Air Working Group Emission Inventory	Lower Athabasca Region of Alberta	2009-2010
Lower Athabasca Regional Plan (LARP) Emissions Inventory	Lower Athabasca Region of Alberta	2006
Environmental Protection and Enhancement Act (EPEA) Approvals Emissions Data	entire province of Alberta	2010
Alberta Industrial Air Emissions Survey	entire province of Alberta	2010
Alberta Air Emissions Inventory (AAEI)	entire province of Alberta	2006-2008
Canadian National Pollutant Release Inventory (NPRI)	all of Canada	2010
Canadian Air Pollutant Emission Inventory (APEI, (not an AQ-modelling-ready version, NPRI is a subset of APEI)	all of Canada	2010
Wood Buffalo Emissions Inventory	WBEA Airshed Zone of Alberta	2005/2006
Two EPEA Approval Applications / Environmental Impact Assessments (EIA) emissions inventories (Frontier and Voyageur South)	project-specific area coverage (Alberta)	various years

Table S2: Summary of Canadian emission sources used for generating JOSM phase 1 emissions input files.

Data Category	Data Sources
Point/Facility Sources	• 2009-2010 CEMA Inventory for AOSR study area (except VOC, NH_3, PM_{10})
	• 2010 NPRI for rest of the domain
OS Off-road Fleet	• 2009-2010 CEMA Inventory
Fugitive Dust from Major Facility	• 2010 NPRI
Tailings Ponds, Mines and Plant Fugitives	• 2010 facility-total VOC emissions from CEMA scaled by NPRI:CEMA
	• Splitting factors for fugitive VOC emissions for tailings ponds, mines and plants based on 2009-2010 CEMA Inventory
Small & Medium Upstream Oil and Gas (UOG) Sources	• 2006 APEI (projected to 2006 from the 2000 Canadian upstream oil and gas emissions inventory)
Non-Mobile Area Sources	• 2006 APEI
Mobile Sources	• 2006 APEI

Table S3: Summary of Canadian emission sources used for generating JOSM phase 2 emissions input files.

Data Category	Data Sources
Point/Facility Sources	• 2009-2010 CEMA Inventory for AOSR study area (except VOC, NH_3, PM_{10})
	• 2010 NPRI for rest of the domain
	• 2013 preliminary NPRI for AOSR Imperial Kearl facility and for NH_3 emissions
	• SO_2 and NO_x from CEMS measurements for stacks of the OS facilities during study period
	• SO_2 from CNRL daily reports during one-week period in August 2013
OS Off-road Fleet	• 2009-2010 CEMA Inventory
Fugitive Dust from Major Facility	• 2013 preliminary NPRI
Tailings Ponds, Mines and Plant Fugitives	• 2010 facility-total VOC emissions from CEMA scaled by NPRI:CEMA
	• Splitting factors for fugitive VOC emissions for tailings ponds, mines and plants based on 2009-2010 CEMA Inventory
Small & Medium UOG Sources	• 2010 APEI (projected to 2010 from the 2000 Canadian UOG emissions inventory)
Non-Mobile Area Sources	• 2010 APEI
Mobile Sources	• 2010 APEI

Table S4: Annual facility-total CO, NO_x, PM_{10}, $PM_{2.5}$, and SO_2 off-road vehicle tail-pipe emissions (tonnes) from 2010 CEMA inventory. These emissions were used for all three phases. (Note: a) PM_{10} emissions were estimated based on the $PM_{2.5}$ emissions and the typical PM_{10} to $PM_{2.5}$ ratio for similar type of off-road vehicles; b) emissions for the Imperial Oil Kearl facility were estimated based on mined oil sands statistics for 2013; and c) off-road VOC emissions are included in this table because they are not included in Table 1 as they are not required for NPRI reporting.)

Facility Name	CO	NO_X	PM_{10}	$PM_{2.5}$	SO_2	VOC
Suncor Millenium/Steepbank	9,087	10,768	484	444	62	1,173
Syncrude Mildred Lake	1,931	8,030	194	178	365	332
Syncrude Aurora North	1,341	7,045	159	146	117	219
Shell Muskeg River/Jackpine	4,577	6,935	225	206	128	653
CNRL Horizon	602	5,585	38	35	66	134
Imperial Oil Kearl	505	1,258	33	30	26	75
Total	**18,042**	**39,620**	**1,132**	**1,039**	**763**	**2,585**

Table S5: Annual facility-total CO, NH_3, NO_x, PM_{10}, $PM_{2.5}$, and SO_2 emissions (tonnes) from stacks and area sources, except for road dust emissions from the off-road mining fleet, by phase for the three phases (P1, P2, P3).

Species & Phase / Facility Name		Suncor Millenium/ Steepbank	Syncrude Mildred Lake	Syncrude Aurora North	Shell Muskeg River/Jackpine	CNRL Horizon	Imperial Oil Kearl	TOTAL
CO	P1	3,080	5,196	883	107	2,785	0	**12,051**
	P2	3,080	5,196	883	107	2,785	484	**12,535**
	P3	6,096	5,184	343	57	1,353	484	**13,517**
NH_3	P1	0	0	0	0	0	0	**0**
	P2	1	1,436	0	0	174	0	**1,612**
	P3	1	1,436	0	0	174	0	**1,612**
NO_X	P1	11,526	14,003	561	696	1,841	0	**28,629**
	P2	11,526	14,003	561	696	1,841	256	**28,884**
	P3	7,848	13,900	519	1,064	1,472	256	**25,059**
PM_{10}	P1	804	4,166	69	26	243	0	**5,308**
	P2	804	4,166	69	26	243	75	**5,382**
	P3	564	2,221	8	35	195	75	**3,098**
$PM_{2.5}$	P1	460	1,538	69	23	243	0	**2,332**
	P2	460	1,538	69	23	243	73	**2,406**
	P3	340	635	7	19	158	73	**1,233**
SO_2	P1	20,619	77,120	0	0	6,512	0	**104,251**
	P2	20,619	77,120	0	0	6,512	0	**104,251**
	P3	13,868	63,321	0	0	4,005	0	**81,194**

Table S6: Annual facility-total PM_{10} and $PM_{2.5}$ fugitive dust emissions from the off-road mining fleet (tonnes) for the three phases.

Facility Name		Suncor Millenium/ Steepbank	Syncrude Mildred Lake	Syncrude Aurora North	Shell Muskeg River/Jackpine	CNRL Horizon	Imperial Oil Kearl	TOTAL
PM_{10}	P1	4,086	1,958	1,702	972	1,642	0	**10,361**
	P2	4,667	2,091	954	2,330	2,099	8,236	**20,377**
	P3	4,667	2,091	954	2,330	2,099	8,236	**20,377**
$PM_{2.5}$	P1	409	196	170	97	164	0	**1,037**
	P2	467	209	95	233	210	2,921	**4,134**
	P3	467	209	95	233	210	2,921	**4,134**

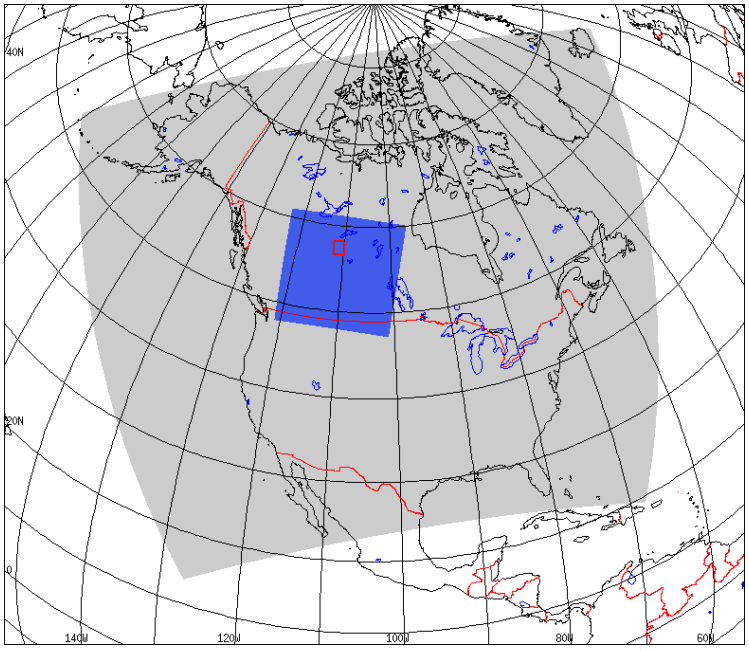

Figure S1: Locations of the North American continental model grid with 10-km grid spacing (grey), the OS western Canada grid with 2.5-km grid spacing (blue), and the subgrid shown in Figures 5 and 7 (red).

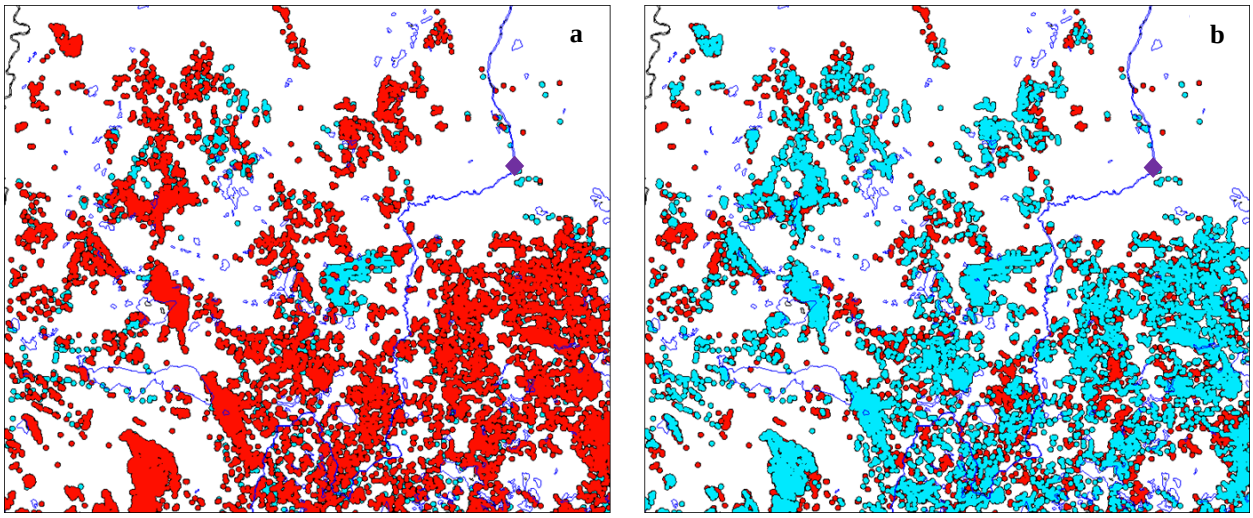

Figure S2: Location of UOG facilities in the vicinity of the Fort McMurray AOSR area from (a) the 2011-based projected 2013 inventory (red dots) superposed on the 2000-based projected 2010 inventory (cyan dots) and (b) the 2000-based projected 2010 inventory (cyan dots) superposed on the 2011-based projected 2013 inventory (red dots). In panel (a) the cyan dots not covered by the red dots are facilities that were in the projected 2010 inventory, but not in the projected 2013 inventory, whereas in panel (b) the red dots not covered by the cyan dots are facilities that were in the projected 2013 inventory, but not in the projected 2010 inventory. The location of Fort McMurray is marked by the purple diamond symbol.

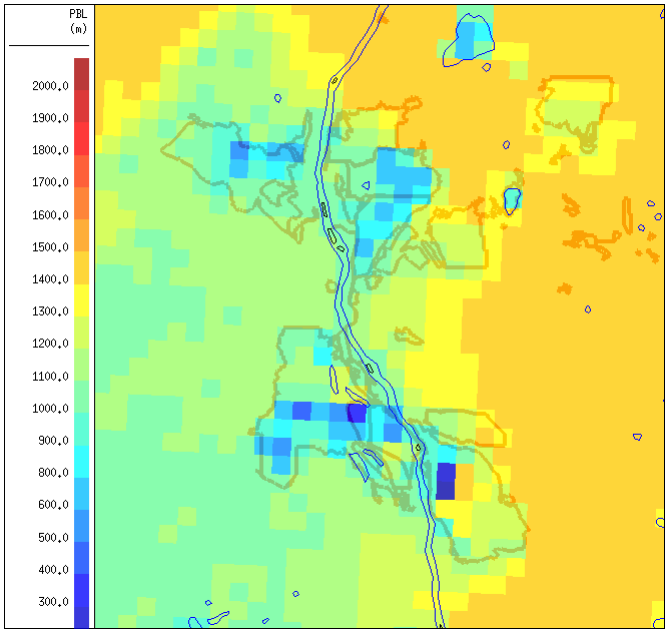

Figure S3: Planetary boundary layer (PBL) height predicted by GEM-MACH using the modified land cover data. The thick grey lines mark the boundaries of the OS facilities and the thin blue lines mark the boundar of natural lakes.

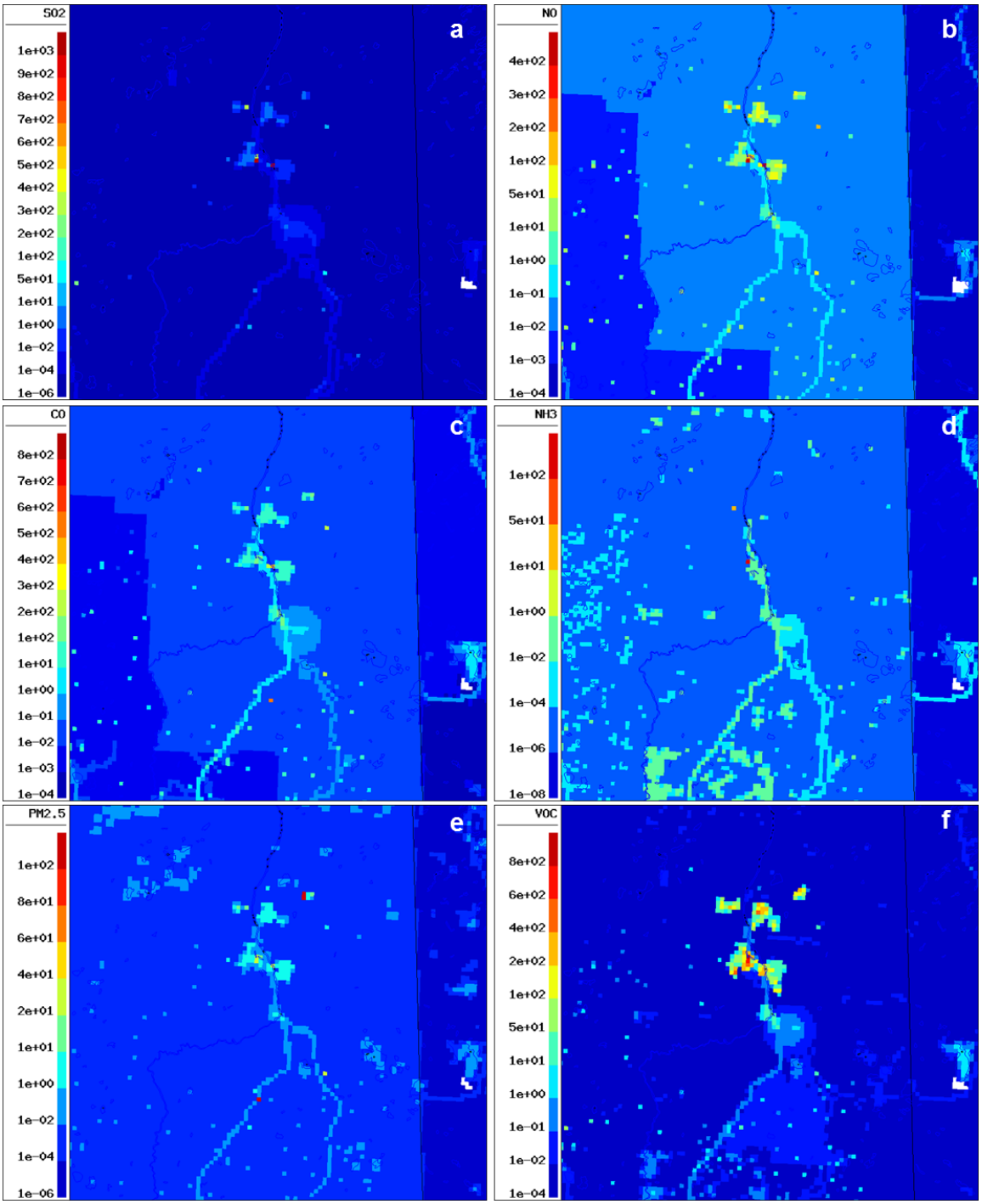

Figure S4: Phase 3 August monthly emissions fluxes (tonnes month^{-1} grid-cell^{-1}) on an interior portion of the OS 2.5-km grid centred on the AOSR study area of the following GEM-MACH species: (a) SO_2; (b) NO; (c) CO; (d) NH_3; (e) $PM_{2.5}$; and (f) VOC.

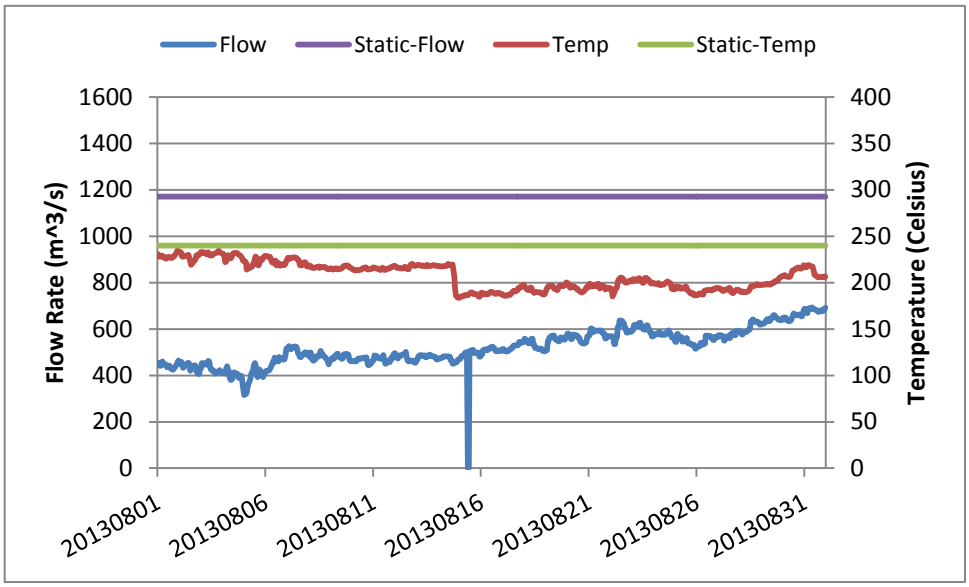

Figure S5: CEMS-measured hourly and NPRI static exit temperature (°C) and volume flow rate (m^3s^{-1}) for the Main stack of the Syncrude Mildred Lake facility for August 2013. Note that CEMS measurements are not available for some hours due to instrument calibration or other interruptions (e.g., flow rate on August 15). Those missing data have been filled by averaging the available data before and after the missing hours.

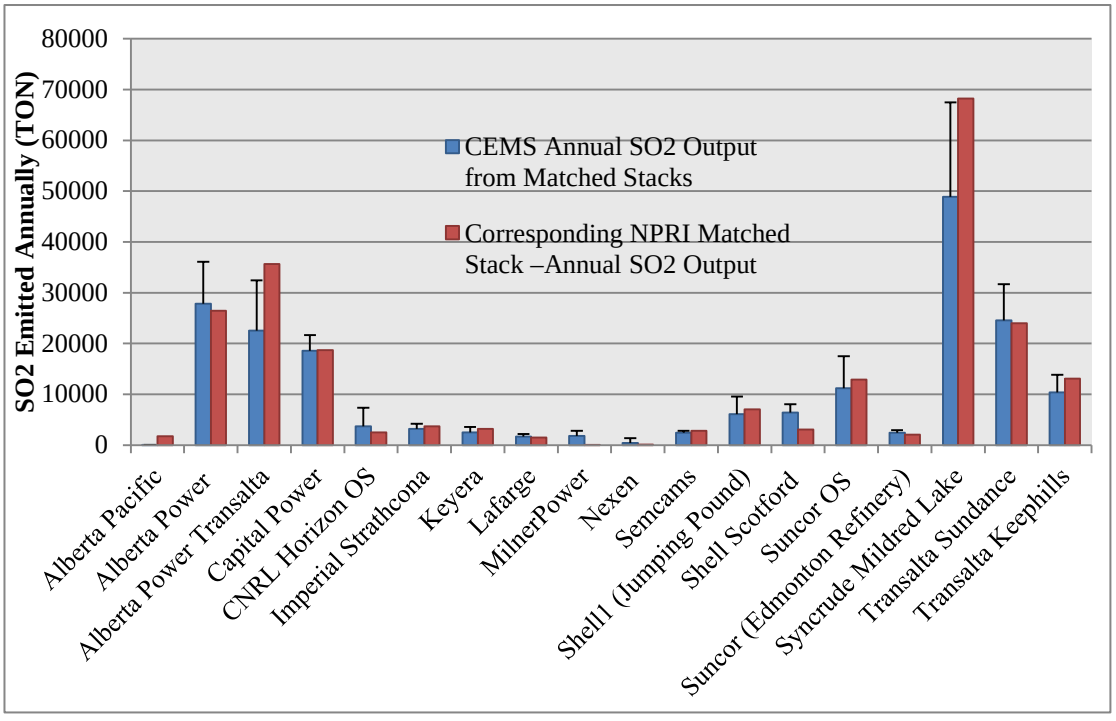

Figure S6: Comparison of annual SO_2 emissions estimated from CEMS measurements at 18 facilities and reported to NPRI for 2013. The error bars shown on the CEMS data represent the standard deviation of the hourly CEMS data measured for August and September, 2013.

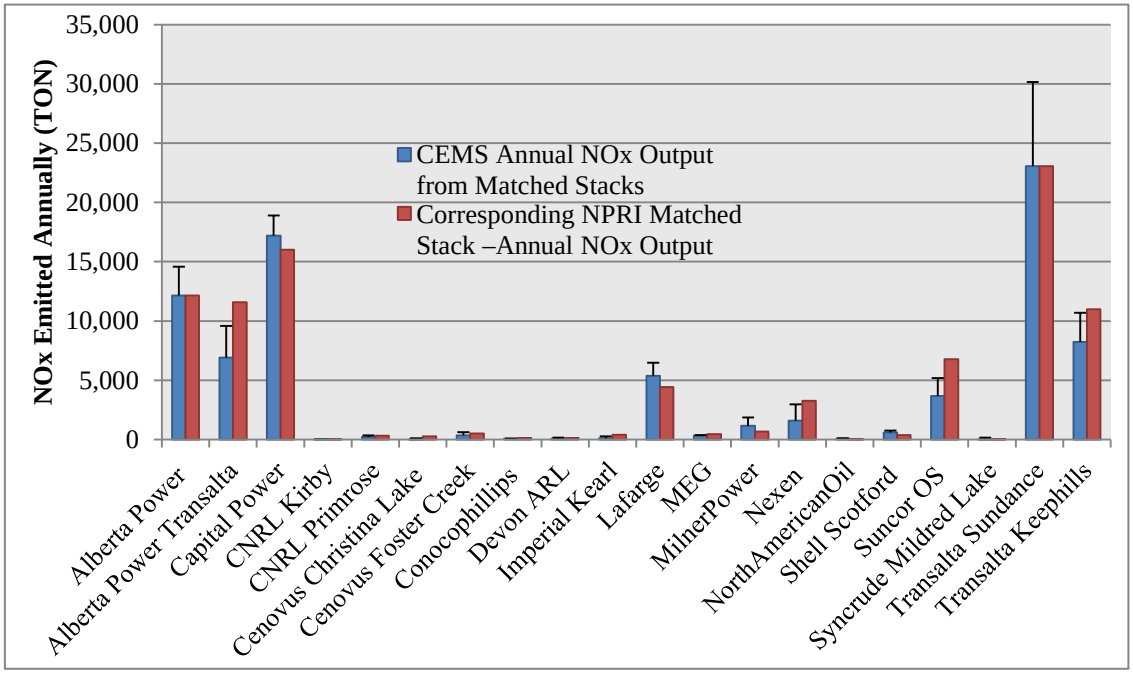

Figure S7: Same as Figure S5, but for NOx comparison and 20 facilities.

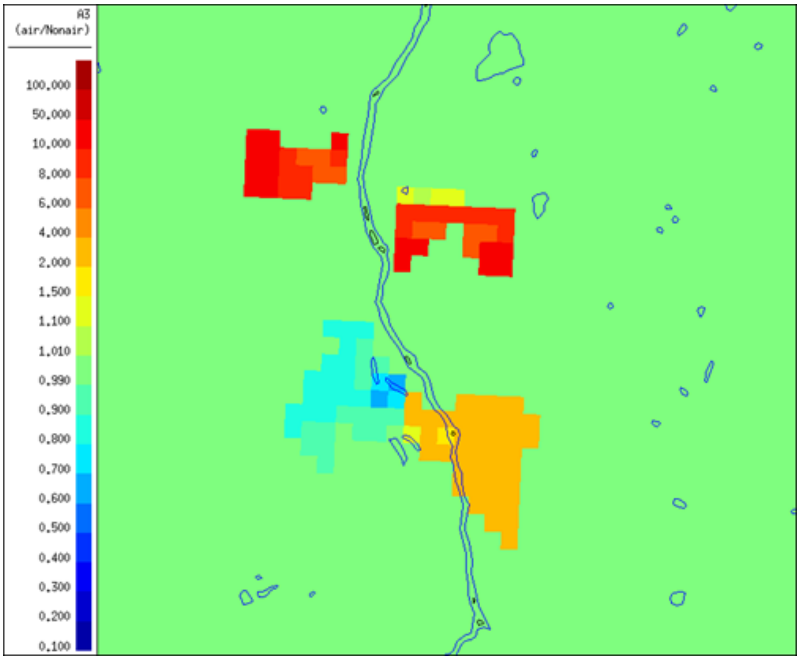

Figure S8: Ratio of gridded model-ready aircraft-observation-based ADOM-2 higher-alkane emissions (top-down) to the base-case emissions (bottom-up) for the GEM-MACH 2.5-km grid over the AOSR area.

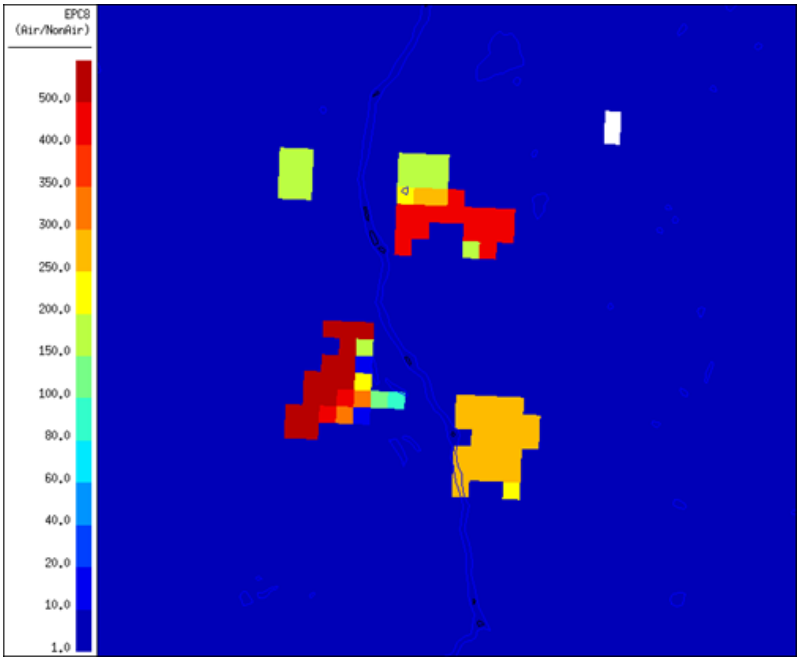

Figure S9: Ratio of gridded, model-ready aircraft-observation-based (size) bin 8 OM emissions to the base-case emissions for the GEM-MACH 2.5-km grid over the AOSR study area.

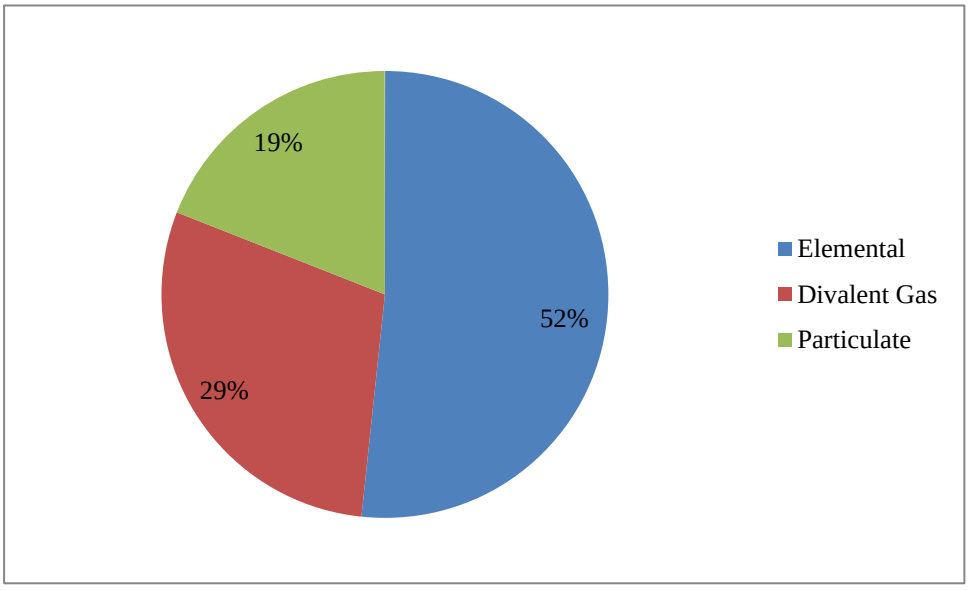

Figure S10: Domain-average percentages of the three speciated mercury species for phase 3 emissions.