Supplement for:

Emissions Preparation and Analysis for Multiscale Air Quality Modelling over the Athabasca Oil Sands Region of Alberta, Canada

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Table S1: List of acronyms used in paper.

AAEI	Alberta Air Emissions Inventory
ADOM-2	Acid Deposition and Oxidant Model, version 2
AEP	Alberta Environment and Parks (formerly AESRD)
AER	Alberta Energy Regulator
AESRD	Alberta Environment and Sustainable Resource Development (now AEP)
AOSR	Athabasca Oil Sands Region
APEI	Air Pollutant Emission Inventory
AQ	air quality
BEIS	Biogenic Emission Inventory System
BELD	Biogenic Emissions Landuse Database
CAC	criteria air contaminants
CEMA	Cumulative Environmental Management Association
CEMS	Continuous Emission Monitoring System
CNRL	Canadian Natural Resources Limited
ECCC	Environment and Climate Change Canada
EIA	environmental impact assessment
EPA	Environmental Protection Agency (U.S.)
EPEA	Environmental Protection and Enhancement Act (Alberta)
GEM-MACH	Global Environmental Multiscale model – Modelling Air-quality and Chemistry
GIS	geographic information system

JOSM	Joint Oil Sands Monitoring plan
LAI	Leaf Area Index
LARP	Lower Athabasca Regional Plan
NEI	National Emissions Inventory
NPRI	National Pollutant Release Inventory
OS	oil sands
PM	particulate matter
SCC	Source Classification Code
SMOKE	Sparse Matrix Operator Kernel Emissions
TERRA	Top-Down Emission Rate Retrieval Algorithm
UOG	upstream oil and gas
VOC	volatile organic compound
WBEA	Wood Buffalo Environmental Association

Table S2: 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 S3: Annual facility-total CO, NOx, 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 2 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 S4: Annual facility-total CO, NH_3, NOx, 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 S5: Annual facility-total PM10 and PM2.5 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**

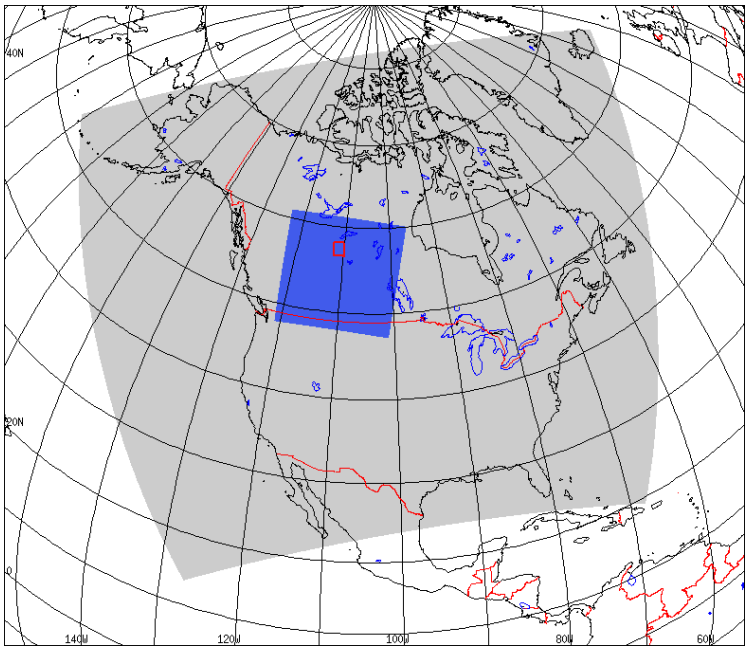

Figure S1: Locations of the North American continental model grid with 10-km grid spacing (grey), the OS western Canada grid with 2.5-km grid spacing (blue), and the subgrid shown in Figures 5 and 7 (red).

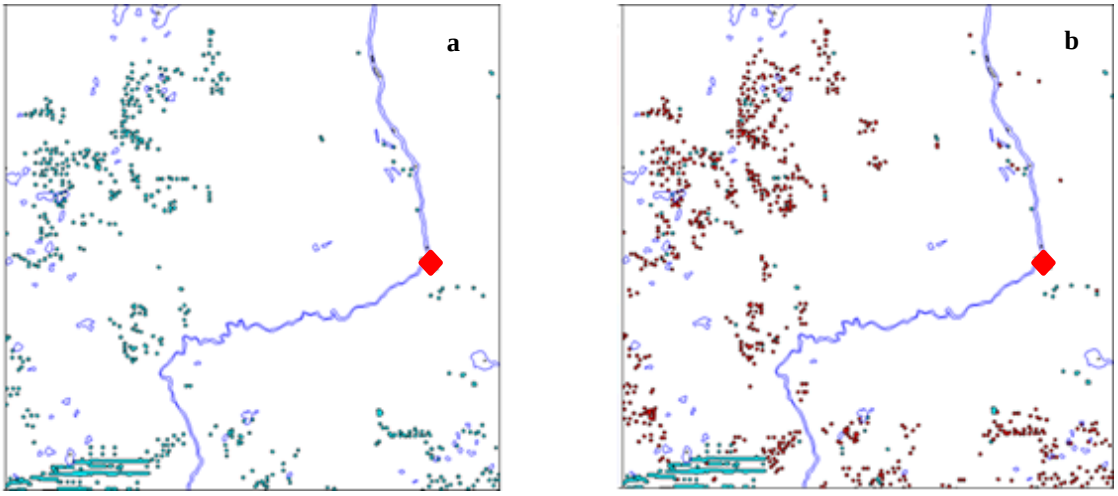

Figure S2: Location of UOG facilities in the Fort McMurray AOSR area from (a) the 2000-based projected 2010 inventory and (b) the 2011-based projected 2013 inventory (red dots) superposed on the 2000-based projected 2010 inventory (cyan dots). The location of Fort McMurray is marked by the diamond symbol.

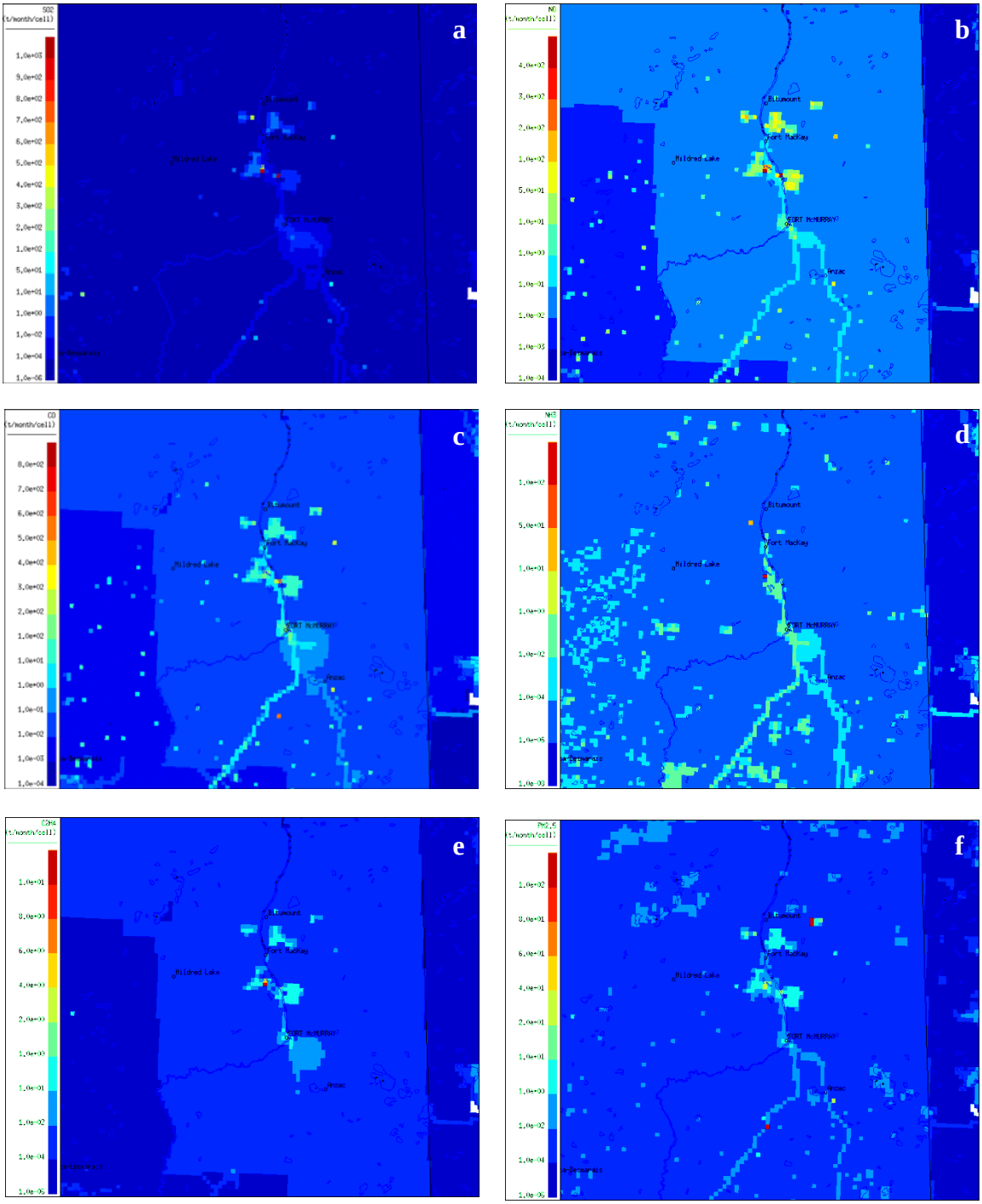

Figure S3: Phase 3 August monthly emissions fluxes (tonnes month^{-1} grid-cell^{-1}) on an interior portion of the OS 2.5-km grid centred on the AOSR study area of the following GEM-MACH species: (a) SO_2; (b) NO; (c) CO; (d) NH_3; (e) $PM_{2.5}$; and (f) C_2H_4 (ethene or ethylene).

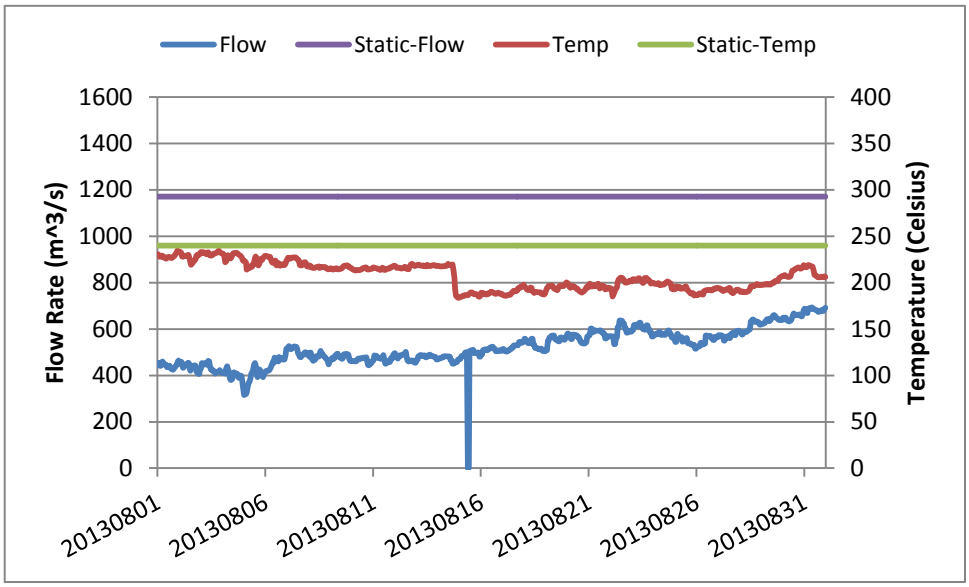

Figure S4: CEMS-measured hourly and NPRI static exit temperature (°C) and volume flow rate (m^3s^{-1}) for the Main stack of the Syncrude Mildred Lake facility for August 2013. Note that CEMS measurements are not available for some hours due to instrument calibration or other interruptions (e.g., flow rate on August 15). Those missing data have been filled by averaging the available data before and after the missing hours.

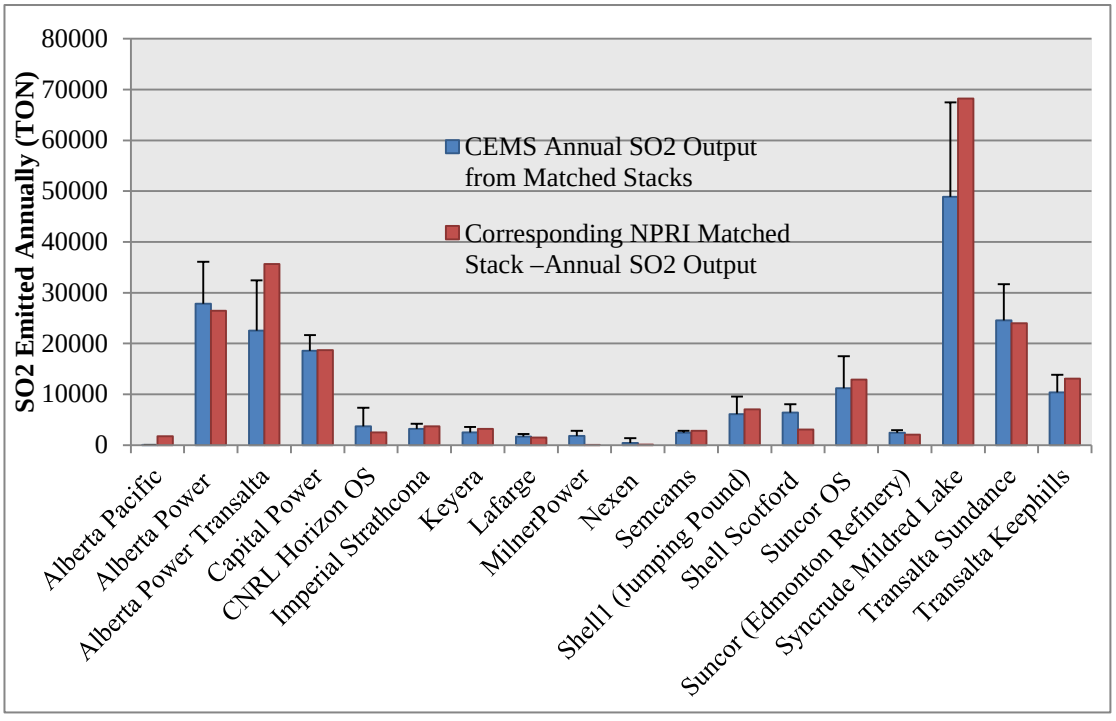

Figure S5: Comparison of annual SO_2 emissions estimated from CEMS measurements at 18 facilities and reported to NPRI for 2013. The error bars shown on the CEMS data represent the standard deviation of the hourly CEMS data measured for August and September, 2013.

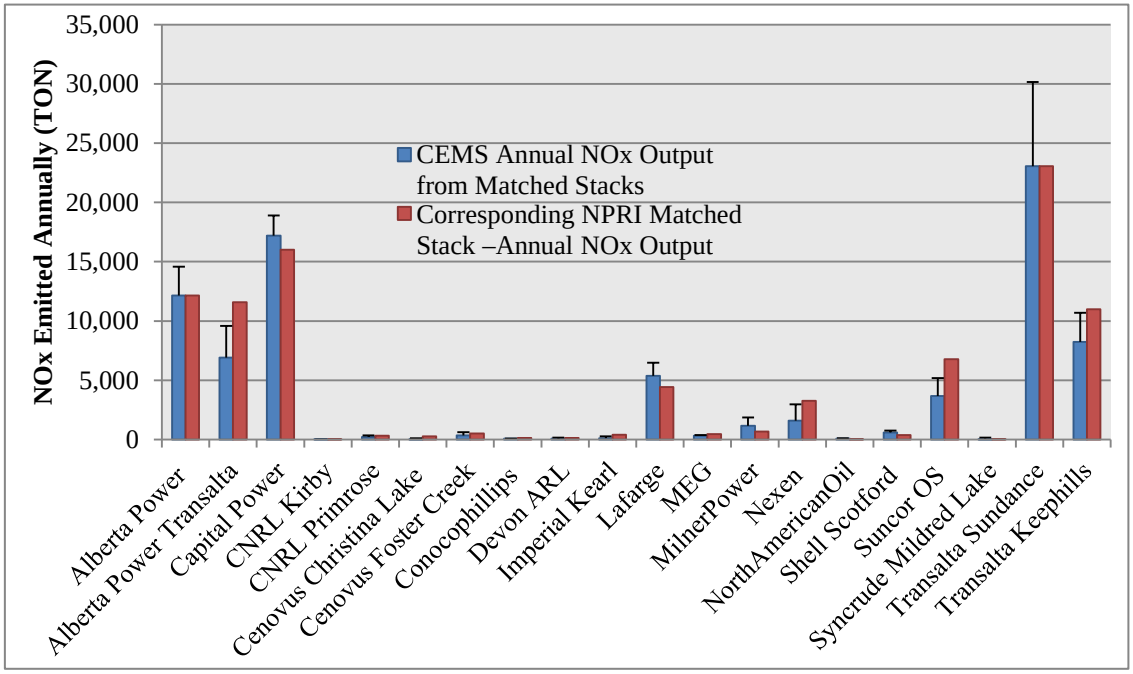

Figure S6: Same as Figure S5, but for NOx comparison and 20 facilities.

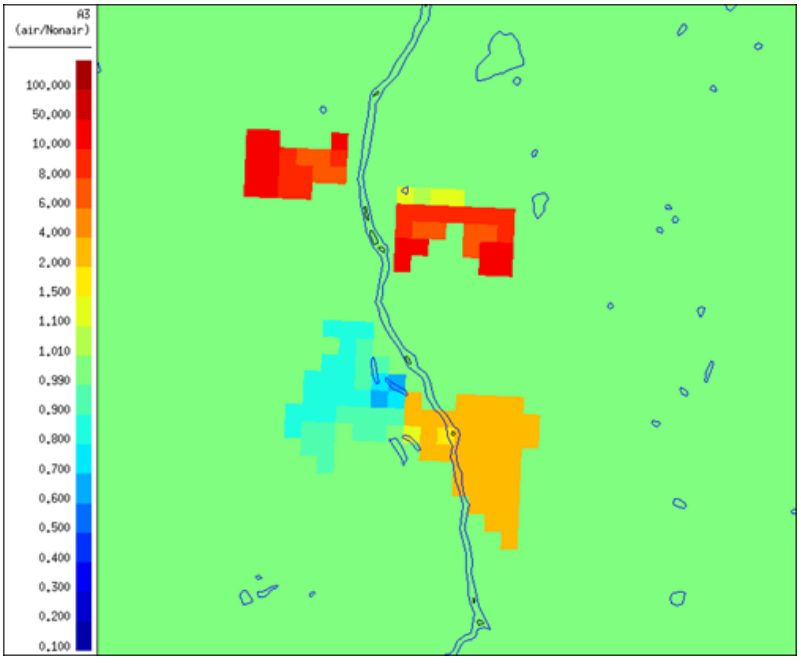

Figure S7: Ratio of gridded model-ready aircraft-observation-based ADOM-2 higher-alkane emissions to the base-case emissions for the GEM-MACH 2.5-km grid over the AOSR area.

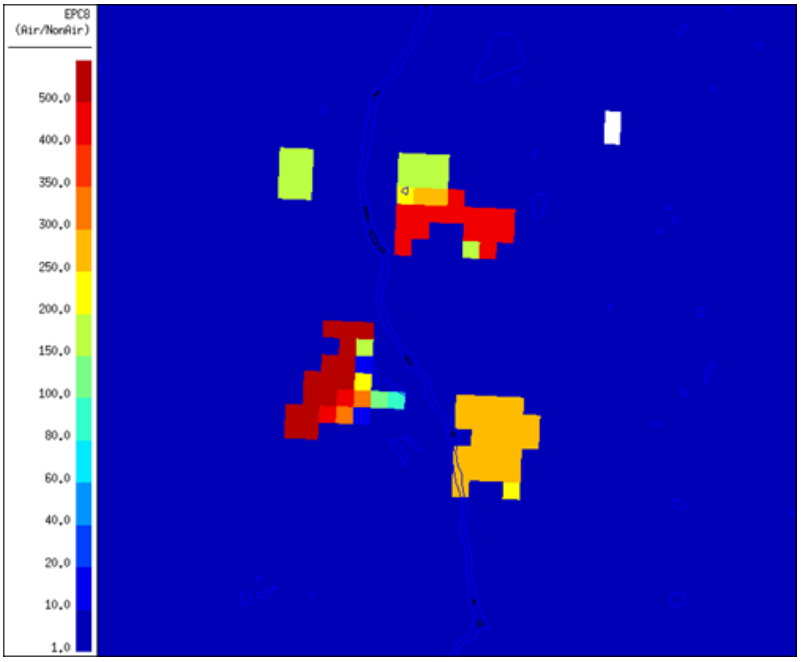

Figure S8: Ratio of gridded, model-ready aircraft-observation-based (size) Bin 8 OM emissions to the base-case emissions for the GEM-MACH 2.5-km grid over the AOSR study area.

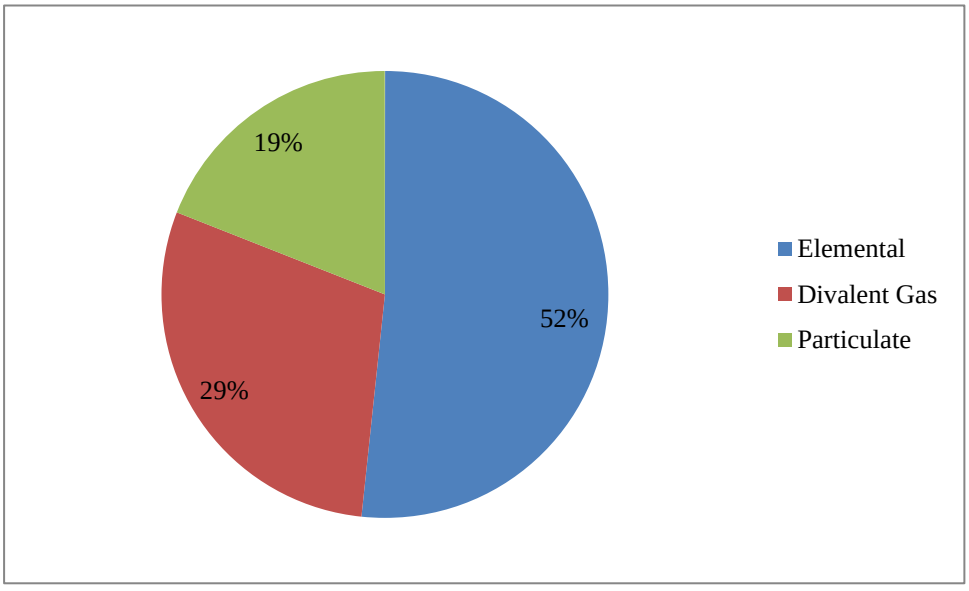

Figure S9: Domain-average percentages of the three speciated mercury species for Phase 3 emissions.