Emissions Preparation for High-Resolution Air Quality Modelling over the Athabasca Oil Sands Region of Alberta, Canada

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ABSTRACT

This paper discusses emissions file preparation for Environment Canada's Global Environmental Multiscale – Modelling Air-quality and CHemistry (GEM-MACH) air quality (AQ) modelling system to conduct nested AQ forecasts during a field study carried out in summer 2013, as well as post-campaign modelling and analysis. This work was performed in support of the Joint Oil Sands Monitoring (JOSM) Plan, a joint initiative between the governments of Alberta and Canada launched in 2012. The study area is located in the Athabasca Oil Sands Region (AOSR) of northeastern Alberta, Canada. The main purpose of the field study was to improve the understanding and assessment of cumulative impacts caused by industrial development activity in Alberta's oil sands. The main focus of this paper is on the development of model-ready emissions input files, for a model domain at 2.5-km resolution centered over the AOSR. For this purpose, multiple emissions inventories covering the study area that had been compiled recently for various applications were reviewed. Additional emission sources, such as emissions measured by Continuous Emission Monitoring Systems (CEMS) and measurements during abnormal operating conditions, were considered for the compilation of a detailed 2013-specific emissions inventory. To account for the large spatial extent of the AOSR mining facilities and the high model resolution, a set of facility-specific spatial surrogates were generated for allocating emissions within each AOSR mining facility. Facility-specific temporal profiles and VOC speciation profiles were also developed. These efforts have resulted in an improved emissions inventory in the study area for the JOSM project. Emissions estimation from aircraft observations made during the field campaign and potential improvements to emissions processing are also discussed.

INTRODUCTION

Oil sands (OS) are a mixture of sand, clay, and water, saturated with bitumen which can be extracted and further upgraded into high-quality, sweet light crude oil. About 71% of global oil sands reserves are found in the province of Alberta, Canada and they are the third-largest proven crude oil reserves in the world (http://www.energy.alberta.ca/oilsands/791.asp, http://en.wikipedia.org/wiki/Oil_reserves). Due to higher oil prices and the availability of new bitumen extraction technology, the extraction and processing of crude oil from oil sands has gone through a rapid expansion over the past decade (http://www.energy.alberta.ca/oilsands/791.asp). The potential environmental impact of these emission sources is therefore of interest, hence the need for accurate source-specific emissions data for this region.

To better characterize air quality in the region and provide data for cumulative effects assessment, an intensive air quality (AQ) airborne and ground-based field study was carried out during the summer of 2013 in support of the Joint Oil Sands Monitoring (JOSM) Plan (a joint initiative between the governments of Alberta and Canada). As part of the field campaign and post-campaign studies, Environment Canada's Global Environmental Multiscale – Modelling Air-quality and CHemistry (GEM-MACH) AQ modelling system was set up to conduct nested AQ forecasts at model grid resolutions down to 2.5 km. Considerable effort was invested in the review of different emission sources, compilation of emissions data, and preparation of model emissions input files for multiple grids to support the AQ modelling. Particular attention was paid to emissions in the field study area.

This paper summarizes the development of model emissions files for the 2.5-km model domain centered over the Athabasca Oil Sands Region (AOSR). It contains the following sections: (1) introduction of the study area and emissions requirements; (2) an overview of the review and selection of the most robust and relevant information from various sources, including those from CEMS (Continuous Emission Monitoring System) measurements and measurements during abnormal operating conditions; (3) generation of facility-specific spatial surrogates, temporal profiles, and VOC speciation profiles; and (4) discussions on potential improvements of emissions estimation based on aircraft measurements and of emissions processing. Conclusions are then given in the last section. This paper summarizes the more model specific portions of the emissions creation – full details on the project may be found in a joint technical report entitled "Joint Oil Sands Monitoring Emissions Inventory Compilation Report"[1] being prepared by the governments of Alberta and Canada. Once finalized, it should be publicly available.

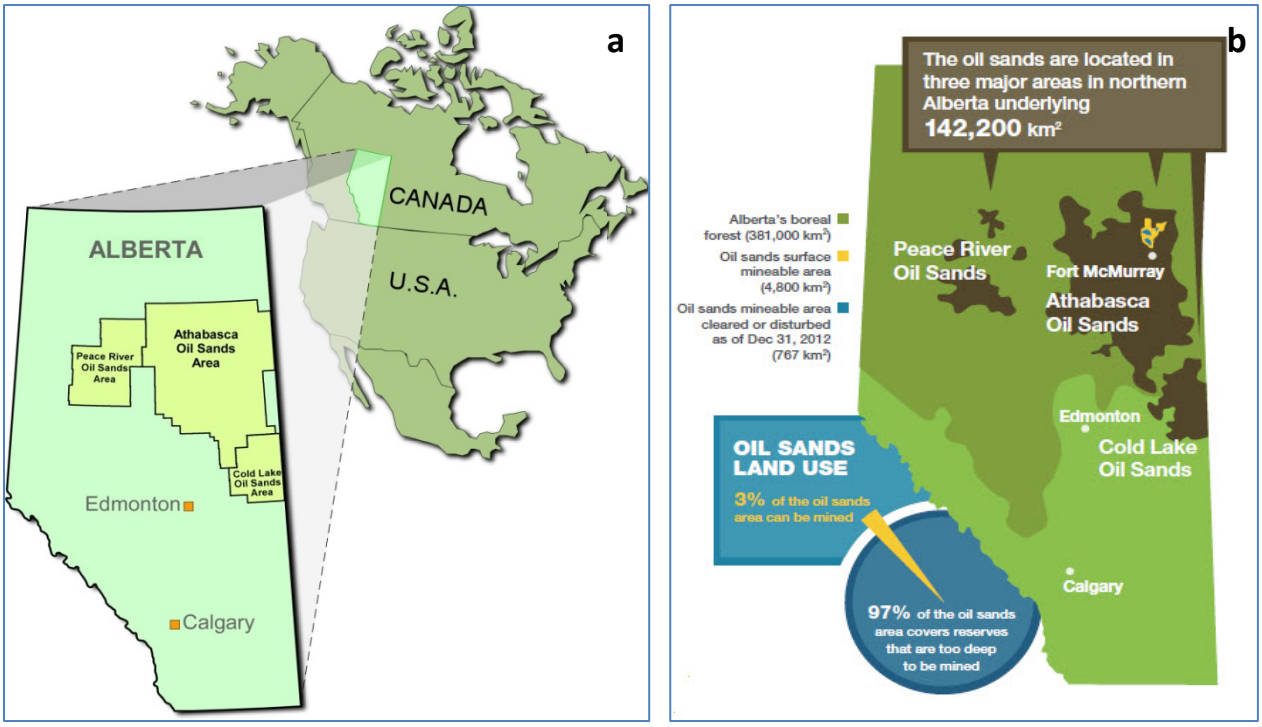
BODY

Study Area and Emissions Requirements

Alberta's oil sands are mainly found in three areas of northern Alberta, the Athabasca, Peace River, and Cold Lake areas, which cover 142,200 km^2 in total (see Figure 1a). The first of these, the Athabasca region, comprises the largest share of oil sands bitumen production. There are two main methods to produce oil from the bitumen in the oil sands, each of which has associated emissions activities. For bitumen that is close to the surface, the oil sands are mined by open-pit mining methods, where large excavators dig up oil sand and transfer it to heavy-hauler trucks for transport to crushers where the large clumps are broken down. This mixture is then thinned with hot water and transported to a processing plant, where the bitumen is separated from the other OS components and upgraded to create synthetic oil. For bitumen that occurs deep within the ground, *in-situ* techniques are used to produce oil (e.g.,

http://www.capp.ca/canadaIndustry/oilSands/Energy-Economy/Pages/what-are-oilsands.aspx). As illustrated in Figure 1b, about 3 per cent of the OS area, which accounts for about 20 percent of the recoverable OS reserves, can be surface-mined, mainly within the AOSR. The remaining 97 per cent of the OS reserves are too deep for surface mining and can only be recovered by *in-situ* methods. (http://www.energy.alberta.ca/oilsands/791.asp).

Figure 1. (a) Location of Alberta's oil sands deposits - the Athabasca, Cold Lake, and Peace River oil sands areas (http://www.ags.gov.ab.ca/energy/oilsands/); and (b) details of the OS deposits and surface mining area (http://www.energy.alberta.ca/oilsands/791.asp).



The oil sands sector is the second largest source of SO_2 and third largest source of industrial NO_X emissions in the province of Alberta[2]. It is also a significant source of industrial PM, CO and VOC emissions. Due to the nature of open-pit mining, pollutants are mainly emitted from the following processes: (1) exhaust emissions from off-road vehicles used for removal of the overburden, excavation, and transportation of the sands to an extraction plant; (2) pollutants emitted from the extraction and upgrading plants; (3) fugitive VOC emissions from mine faces, tailings ponds, and plants; and (4) fugitive dust kicked up by the off-road mine fleets. The emissions from current levels of *in-situ* activities are much smaller than those of current open-pit mines. Therefore, the summer 2013 field study mainly focused on the surface mining area in the AOSR, with some flights designed to study a representative *in-situ* facility. An overview of the study area is shown in Figure 2, where all six of the operating (as of 2013) surface mining facilities are located.

Figure 3 shows the three-level nested GEM-MACH model grids, where the innermost and highest-resolution grid, with 2.5-km horizontal grid spacing, is centered over the study area. The outermost and largest GEM-MACH grid covers most of North America with 10-km grid spacing. It provides initial and boundary conditions to an embedded 10-km middle grid that covers most of western Canada and the north-western portion of the contiguous U.S. This middle grid employs the same physical parameterizations as the innermost grid and it provides initial and boundary conditions for the 2.5-km grid, which covers most of the provinces of Alberta and Saskatchewan.

Figure 2. Overview of the 2013 summer field study area (adopted and modified from Li et al., 2014)[3].

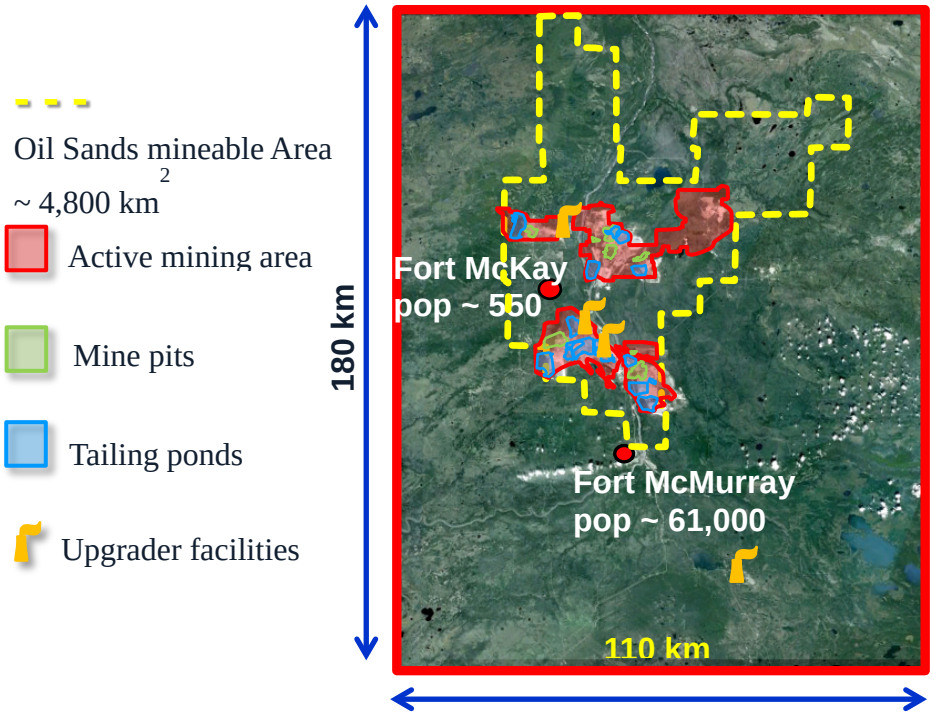
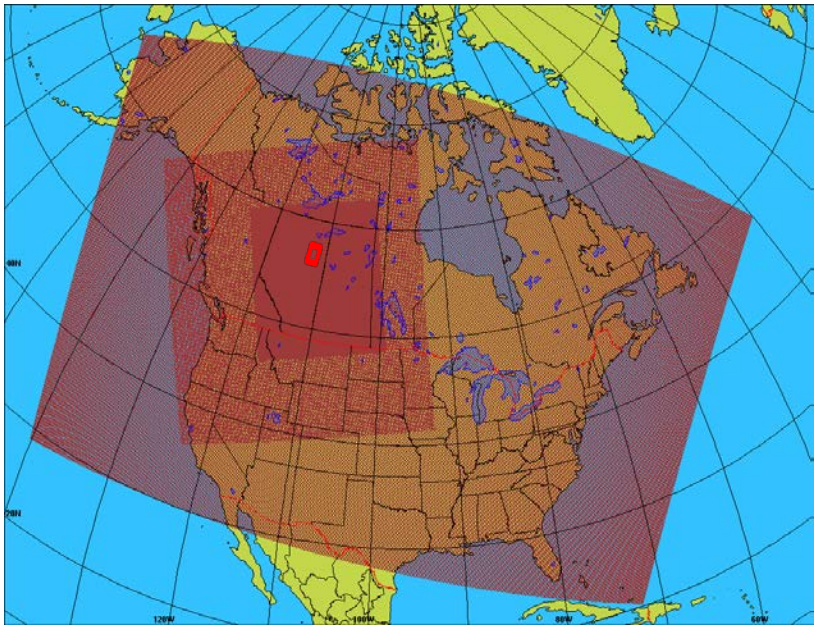


Figure 3. Three-level nested grids of GEM-MACH used for the OS experimental forecasts, the summer 2013 field study, and post-campaign analysis. The red box marks the location of the study area indicated in Figure 2.



The goal of this emissions preparation exercise was to use the best available information from existing emissions inventories and related sources in order to provide emissions that are as accurate and representative as possible for the 2.5-km and two 10-km GEM-MACH grids. GEM-MACH in turn was used to provide near-real-time AQ forecast guidance for airborne laboratory flight planning during the 2013 summer field study, aid in the subsequent analysis and interpretation of the field-study measurements, and provide inputs for ongoing experimental forecasts of air-quality on the same domains.

Review of inventories and other information sources

Over the years, many emission inventories that cover the study area have been developed for various purposes. The inventories that were considered to be the most recent and relevant to this study were reviewed extensively, in order to select the most appropriate inventory or synthesis of multiple inventories to meet the requirements of AQ modeling for the field study[1,4,5]. This section highlights the main findings of this inventory review activity.

Listed below are the nine emissions inventories that were reviewed. Their geographic coverage and levels of detail are summarized in Table 1.

- The Cumulative Environmental Management Association (CEMA) Air Working Group Emission Inventory;
- The Lower Athabasca Regional Plan (LARP) Emissions Inventory;
- Environmental Protection and Enhancement Act (EPEA) Approvals Emissions Data;
- The Alberta Industrial Air Emissions Survey;
- The Alberta Air Emissions Inventory (AAEI);
- The Canadian National Pollutant Release Inventory (NPRI) from industrial, commercial, institutional and other facilities that meet certain reporting requirements;
- The Canadian Air Pollutant Emissions Inventory (APEI: NPRI is a subset of APEI);
- The Wood Buffalo Emissions Inventory;
- Two EPEA Approval Applications / Environmental Impact Assessments (EIA) emissions inventories (Frontier and Voyageur South)

Table 1. The geographic coverages and levels of detail of the nine reviewed inventories.

Inventory Name	**Geographic Coverage**	**Level of Detail**
CEMA Inventory	Lower Athabasca Region	Release-point level (e.g., stack)
LARP Inventory	Lower Athabasca Region	Release-point level (e.g., stack)
EPEA Approvals	Entire Province	Facility total, some release-point
Alberta Industrial Air Emissions Survey	Entire Province	Release-point level (e.g., stack)
AAEI	Entire Province	Facility total, some release-point
NPRI (subset of APEI)	All of Canada	Facility total, some release-point
APEI	All of Canada	Sector category totals for the whole province
Wood Buffalo Emissions Inventory	Wood Buffalo Environmental Association Airshed Zone	Release-point level (e.g., stack)
EPEA Approval Applications & EIAs	Variable, project-specific	Release-point level (e.g., stack)

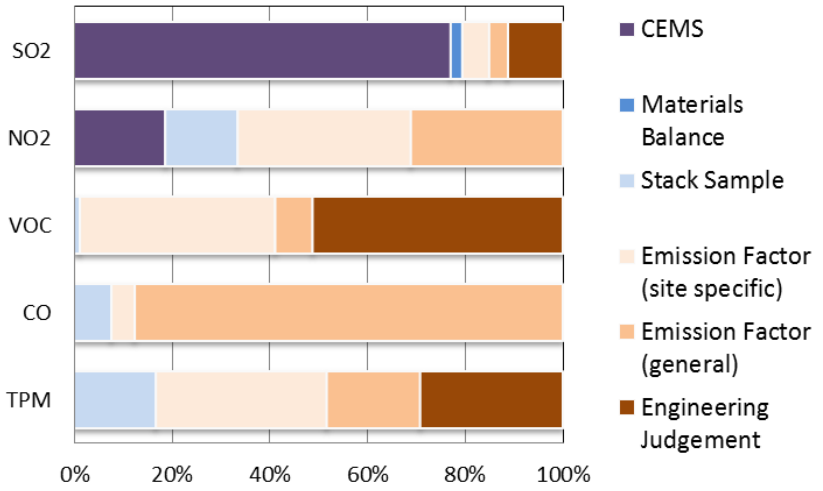
These different emissions inventories were developed with different objectives in mind including: for specific modelling projects, for overall understanding of air emissions in a particular area, for Environment Impact Assessments, or for provincial or national inventory construction. Different inventories also had different base years, and provided different emissions totals for the AOSR, for those inventories which had regional coverage (see Table 2). From Table 2, it can be seen that the differences amongst these inventories are relatively small for some species data collected in common across all inventories, such as SO_2, whereas for other pollutants such as total VOC, the differences can be a factor of two or three. These differences may be due in part to the choice of different inventory years (e.g. 2006 vs. 2009 vs. 2010) and in part to the different purposes for which the inventories were constructed.

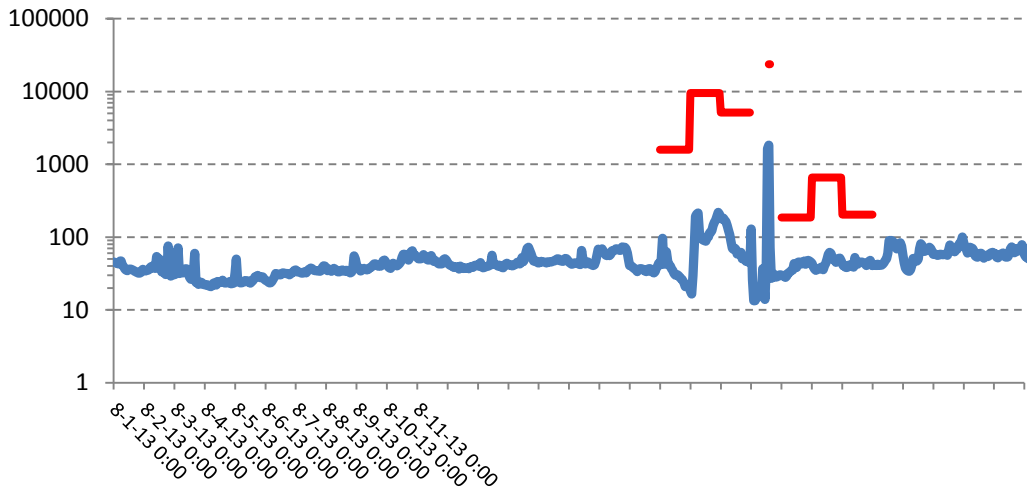
However, it is also likely that some of the differences between the different inventories result from the use of different emissions estimation techniques, with different uncertainties. As an example, Figure 4 shows the different quantification techniques used for estimating the criteria-air-contaminant (CAC) emissions from the AOSR non-conventional oil and gas industry based on a 2008 Industrial Survey conducted by the Alberta Ministry of Environment and Sustainable Resource Development (AESRD)[6]. These techniques are shown from left to right sorted by level of estimation accuracy in descending order; that is, CEMS is expected to be the most accurate and least uncertain and Engineering Judgement is expected to be the least accurate and most uncertain. We can see that SO_2 emissions were obtained mostly from CEMS direct measurements, the technique with the highest expected accuracy. VOC emissions, on the other hand, were estimated mainly by Emission Factors and Engineering Judgement, the two methods with the expected highest uncertainty. These uncertainties contribute to the larger variation in emissions estimates for VOC than SO_2.

Table 2. Comparison of total emissions from AOSR facilities. Inventory base years are indicated in the leftmost column.

Inventory Name	NOx (tonnes / year)	SO_2 (tonnes / year)	CO (tonnes / year)	PM2.5 (tonnes / year)	VOC (tonnes / year)
CEMA Total Oil Sands (2009/2010)	81,125	115,746	42,669	4,482	32,292
LARP Total Oil Sands (2006)	83,246	113,886	51,317	5,857	80,648
EPEA Approvals Total Oil Sands (2010)	66,839	113,550	-	-	-
Alberta Industrial Survey Total Oil Sands (2008)	63,164	117,819	25,875	3,896	47,176
AAEI Oil Sands Facilities in LARP (2008)	62,621	107,185	25,413	3,871	46,044
NPRI Oil Sands *In-Situ* Extraction and Processing + Oil Sands Mining Extraction and Processing + Bitumen and Heavy Oil Upgrading Sector Totals (2010), Excluding Mine Fleets	44,318	113,138	24,075	2,003	73,835
APEI Total Alberta Oil Sands, including NPRI and mine fleet (2010)	94,167	113,150	59,643	3,699	77,859

Figure 4. Quantification methods used for building emissions inventory for non-conventional oil and gas industry based on a 2008 AESRD industrial survey.

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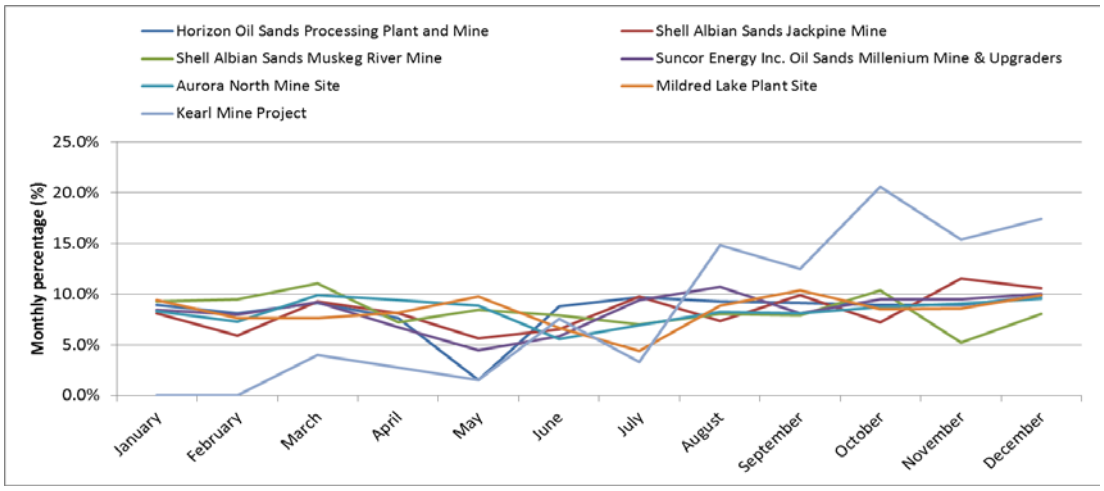
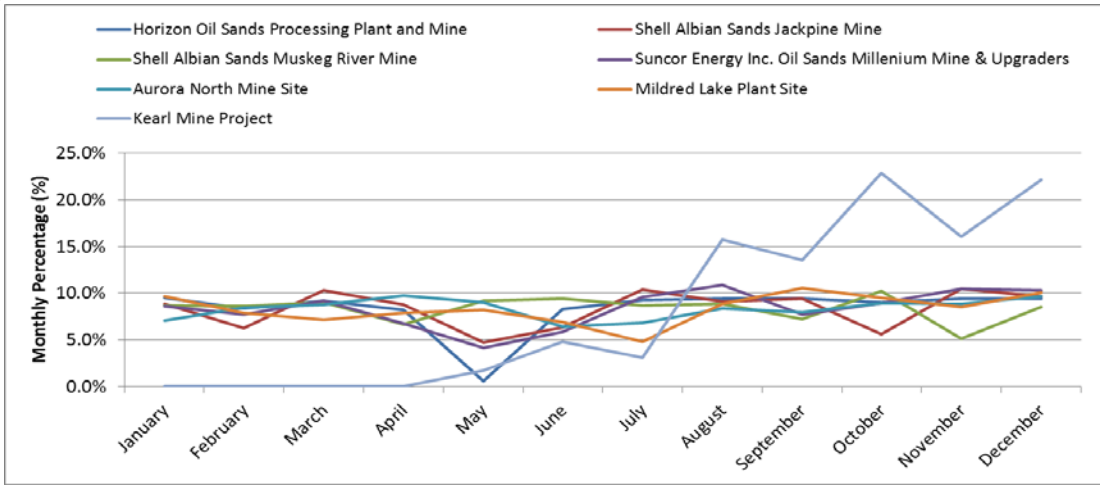
Since the off-road fleets at each OS facility are mainly used for mining activities, the Mined Sands statistics are considered to be a good proxy to build monthly temporal profiles for off-road fleet emissions for each of the six facilities as shown in Figure 11. Again, note that the two Shell Albian Sands mines are shown here separately but they were combined to create a single monthly temporal profile for emissions processing due to the fact that they are treated as one facility in the emissions inventory. These monthly profiles are also used for temporal allocation of fugitive dust emissions for each facility, since dust kicked up by the off-road mine fleets is the main source of fugitive dust emissions.

Figure 11. 2013 monthly temporal profiles created for off-road emissions according to mined-oil-sands statistics. (Note that the Shell Albian Sands Jackpine mine and Muskeg River mine profiles were subsequently combined into a single profile for emissions processing.)



In a similar fashion, monthly temporal profiles for plant emissions were created, in this case based on 2013 monthly bitumen-production statistics as shown in Figure 12. We can see that these profiles also vary significantly from month to month, similar to the monthly profiles used for off-road emissions. We can also see that although the new Imperial Kearl mine began mining activity in March 2013 (Figure 10), significant amounts of bitumen were first produced two months later, in May 2013, and then production levels gradually increased in the second half of the year.

Figure 12. 2013 monthly temporal profiles created for plant emissions according to bitumen-production statistics, expressed as percent of the annual total emissions. (Note that the Shell Albian Sands Jackpine mine and Muskeg River mine profiles were subsequently combined into a single profile for emissions processing.



For fugitive VOC emissions from tailings ponds and open mine faces, the assumption was made that they are less likely to be production-related, and probably depend mainly on ambient temperature and wind speed. Based on OS EIA submissions (Cenovus – Narrows Lake, UTS/Teck Equinox and Frontier projects), the ambient-temperature-based monthly temporal profile shown in Table 5 was used for processing fugitive VOC emissions from tailings ponds and mine faces.

Table 5. Monthly variation assumptions for VOC emissions from tailings ponds and mine faces based on some OS EIA studies.

Month	Degree-days > 0°C	% diluent loss emitted
January	1.6	2.7
February	5.1	3.4
March	23.1	6.9
April	139.3	29.6
May	322.0	65.3
June	439.9	88.3
July	519.2	100.0
August	474.2	95.0
September	282.4	57.5
October	119.9	25.8
November	7.4	3.8
December	1.4	2.6
Average		**40.1**

Generation of Facility- and Process-Specific VOC Speciation Profiles

Emissions inventories usually report emissions for only a small number of individual and bulk species such as NO_x, VOC, $PM_{2.5}$, and SO_2, whereas the species simulated by an AQ model are often much more detailed. Chemical speciation profiles are therefore used to allocate inventory species to multiple model species, particularly for VOC species. VOC chemical speciation profiles are also dependent on the speciation of organic gases assumed by the model's gas-phase chemical mechanism. Under the 1999 Canadian Environmental Protection Act (http://laws-lois.justice.gc.ca/eng/acts/C-15.31), up to roughly 300 detailed VOC species may be reported to the NPRI by individual facilities. However, these reports are for facility-wide totals. The CEMA inventory, on the other hand, has proposed VOC speciation profiles for a number of process-specific sources of emissions, such as mine faces, various types of processing plants, and tailings ponds[7]. As an example, Table 6 lists six VOC speciation profiles for VOC emissions from different types of tailings ponds from this inventory. We can see that the relative amounts of chemical species vary significantly from pond to pond. Therefore, the CEMA VOC speciation profiles were adopted for VOC speciation, and the mapping from CEMA VOC species to the model VOC species used by the GEM-MACH ADOM-2 (Acid Deposition and Oxidant Model) chemical mechanism is shown in Table 7.

Table 6. CEMA tailings ponds VOC speciation profiles (as percentages of bulk VOC emissions).

Solvent Type (If available)	**Paraffinic**	**Hydrotreated Naphtha**	**Untreated Naphtha**	**N/A**	**N/A**	**N/A**
Tailings Type/ CEMA species	**Primary / Secondary (POND1)**	**Primary / Secondary (POND2)**	**Primary / Secondary (POND4)**	**Primary (POND3)**	**InPit (INPIT)**	**Recycle (POND5)**
Paraffins carbon	54.42	51.33	62.58	55.05	63.31	53.85
Terminal olefin carbon bond (R0.0C=C)	0.47	0.3	7.15	2.42	1.02	11.07
Toluene and other monoalkyl aromatics	0.42	0.71	6.31	10.82	15.94	12.08
Xylene and other polyalkyl aromatics	40.11	44.7	22.46	20.18	14.64	21.16
Formaldehyde	0.05	0	0.079	0.066	0.1	0.081
Acetaldehyde	0.0075	0	0	0.014	0.05	0
Ethene	0	0	0	0	0.0025	0
Isoprene	0.019	0	0	0.0023	0.0008	0.0043
Methanol	0.23	0	0	0.89	0.00041	0
Ethanol	0.0046	0	0	0	0.00033	0
Internal olefin carbon bond (R0.0C=C0.0R)	0.37	0.26	1.04	1.49	0.15	1.29
Propionaldehyde and higher aldehydes	0.24	0.036	0.017	0.24	1.18	0.012
Terpene	0.64	0.11	0	0.15	0.49	0
Total	**96.98**	**97.45**	**99.64**	**91.3**	**96.8**	**99.5**

Table 7. VOC species considered in the CEMA inventory and the mapping to ADOM-2 species.

CEMA VOC Species	**ADOM-2 Species**	**Name of ADOM-2 Species**
Paraffins carbon bond (C0.0C)	>C3 Alkanes	EA3
Terminal olefin carbon bond (R0.0C=C)	>C2 Alkenes	EA2
Toluene and other monoalkyl aromatics	Toluene	ETOL
Xylene and other polyalkyl aromatics	Higher Aromatics	EARO
Formaldehyde	Formaldehyde	EHCH
Acetaldehyde	Acetaldehyde	EALD
Ethene	Ethene	EETH
Isoprene	Isoprene	EISO
Methanol	Propane	EC38
Ethanol	>C3 Alkanes	EA3
Internal olefin carbon bond (R0.0C=C0.0R)	>C2 Alkenes	EA2
Propionaldehyde and higher aldehydes	Acetaldehyde	EALD
Terpene	>C2 Alkenes	EA2

Potential Improvements to Emissions Estimation and Emissions Processing

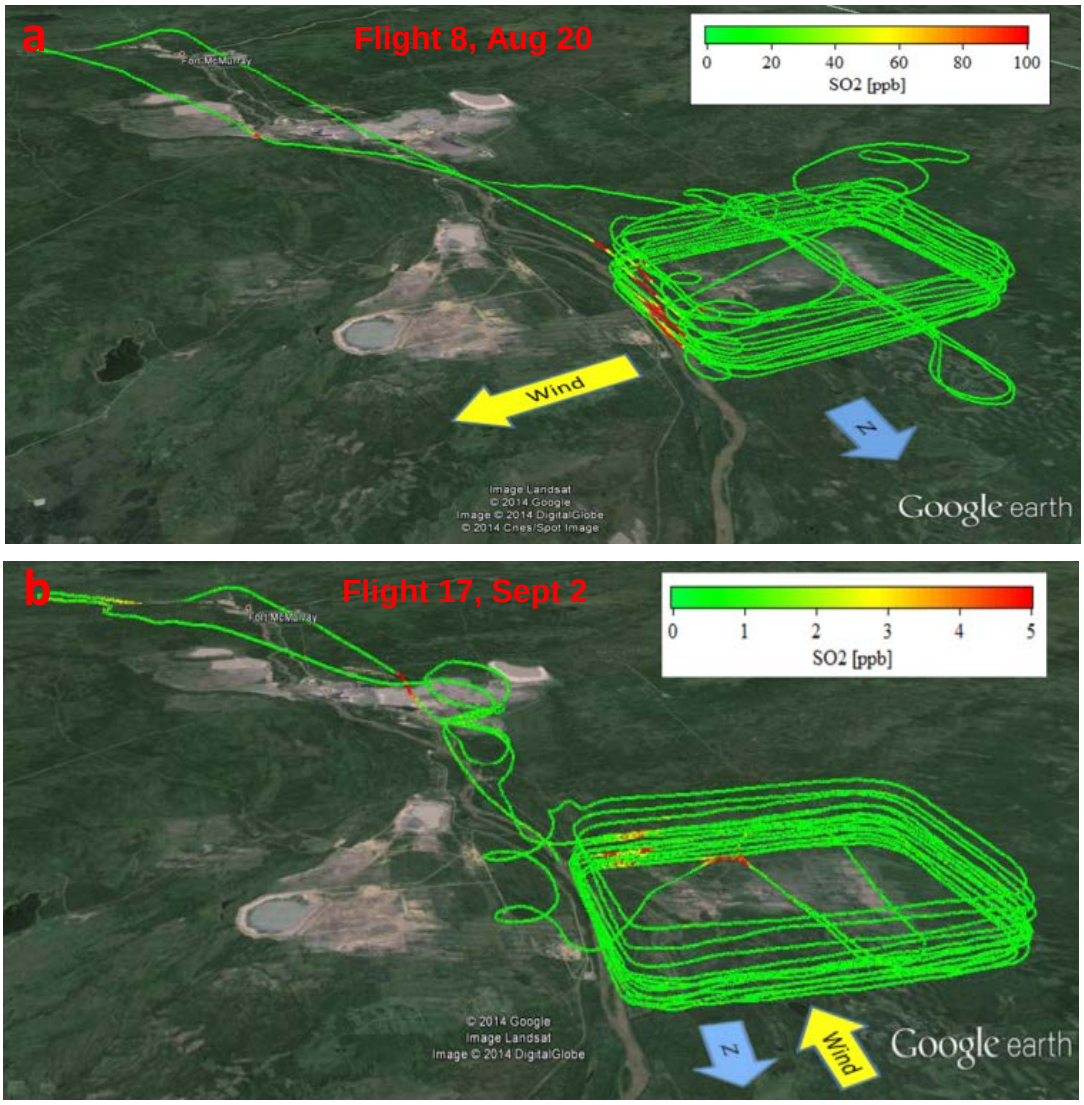
As discussed in the previous sections, there are still large uncertainties associated with emissions inventories. Continuing efforts are required to improve the accuracy of emission estimations. The quantification of emissions of criteria air contaminants (CACs) and other air pollutants through ambient air measurements in the AOSR region was one of the goals of the 2013 summer field study. A total of 22 flights (84 hours airborne) were flown during this study, and a number of these flights were dedicated to emissions estimation. As an example, Figure 13 shows SO_2 concentration measured during two of the flights, one on August 20 (Flight 8) and the other one on September 2 (Flight 17): on both days the flight paths included numerous circuits around the CNRL Horizon facility. The lines plotted in the two panels mark the flight tracks and the colours of the lines represent SO_2 concentrations. For each flight, the aircraft was flown around the facility in a rectangular shape on different levels to form a closed "box" in order to calculate SO_2 mass coming into and leaving the box. This figure shows that much higher SO_2 concentrations were observed on the downwind side of the box than on other three sides. It also shows that the maximum SO_2 concentration observed during Flight 8 on August 20 at the plume center is more than one order of magnitude larger than that observed for the same facility during Flight 17 on September 2. This is consistent with the reports from this facility of abnormal operating conditions on August 20, with a large amount of SO_2 being emitted through the flaring stacks (cf. Figure 5). To calculate emissions from aircraft measurements, a new Top-down Emission Rate Retrieval Algorithm (TERRA) has been developed[8]. Estimates of SO_2 emissions calculated from flight measurements using TERRA are being compared with inventory values. Estimates of other species will also be made, including the use of detailed VOC species concentrations observed by aircraft to evaluate current VOC speciation profiles.

CONCLUSIONS

The use of accurate and representative emissions inventories and emissions processing is important for successful air quality modeling. As an essential first step, emissions inventories should be examined, analyzed, and compared with other existing inventories to understand their strengths and weaknesses before an inventory is chosen and utilized. Emissions processing also needs to be tailored for the target modelling objectives and modelling grid. For this study, rather than treating all industrial facilities as point sources, it was necessary to allocate emissions spatially within some individual facilities due to the large spatial extent of these facilities and the high-resolution modelling grid that was used. Representativeness is also important. The base year of the chosen inventory should match the modelling period as closely as possible, particularly for the OS area, due to its fast development. Chemical speciation is another key component of emissions processing that often has large uncertainties. To reduce this uncertainty, the chemical speciation profiles that are used should be as source-specific as possible.

After a considerable effort to address these requirements, an improved emissions inventory for the study area has been compiled for the JOSM project. While this paper provides an overview and summary of this work, a more comprehensive and detailed description of the inventory compilation and emissions processing preparation work is contained in the references[1]. The resulting JOSM synthesized inventory was used to generate the input emissions files that were used by the GEM-MACH AQ model to provide near-real-time guidance for flight planning during the summer 2013 field study carried out in the AOSR, with subsequent updates being used to improve post-campaign analysis as the observation data are quality assured and controlled. Post-campaign model runs with these improved emissions are now underway to assist in the analysis and interpretation of the field-study measurements. As well, aircraft observations made during the field study are expected to provide valuable information for emissions estimation that may further improve the JOSM inventory.

Figure 13. Aircraft-observed SO_2 concentrations during two flights circling the CNRL Horizon facility: (a) Flight 8 on August 20, 2013; and (b) Flight 17 on September 2, 2013.



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*Note: These draft reports are under review. They should be publicly available once finalized.

KEY WORDS

Emission Inventories
Emission Processing
Oil Sands
Alberta
Spatial Surrogate
Temporal Profile
Chemical Speciation
CEMS
GEM-MACH