

2006 Canadian emissions for air quality modelling

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Abstract

The Air Quality Modelling Applications Section of Environment Canada is developing emissions modelling files to be used for air quality policy scenario assessments. A transition from 2002 to 2006 emissions inventories was recently completed. It involved updates to inventories and surrogates as well as new developments in mobile emissions modelling and improved treatment of particulate matter emissions.

As Canadian area source emissions inventories are published on a provincial level, the accuracy of the final emissions modelling files is very dependent on the quality of the spatial surrogates used. A new set of spatial surrogates were developed based on improved socio-economic data from the 2006 Canadian census. The treatment of PM emissions was also revised. Sector-specific PM size disaggregation into twelve size bins, and Source Classification Code (SCC)-specific chemical speciation for the ADOM-II chemistry mechanism were applied. The generation of the fugitive dust transportable fraction was also revised.

The treatment of mobile emissions benefited from an extensive update to the Canadian version of MOBILE6. The model integrates the latest Canadian measurements to account for recent vehicle technology and bio-fuels use. Additional volatile organic compounds (VOC) from MOBILE6 were used to develop speciation profiles for the ADOM-II mechanism. Emissions sensitivity to fuel composition is an asset for policy scenarios, and was used to study the impact of biodiesel fuels in diesel vehicles. Mobile emissions also have improved spatial and temporal distributions.

1. Introduction

One mandate of the Air Quality Modelling Applications Section (AQMAS) is to deliver modelling scenarios in support of Canadian air quality policy assessments. This is achieved by using an integrating modelling framework, the Canadian Modeling Platform for Policy Emission Reduction Scenarios. The *platform* encompasses all tools used to prepare, document, run and analyze policy modelling scenarios. Emission processing is one critical step of scenario preparation. AQMAS is continuously improving its emission processing methodology in order to provide the best speciation and the best spatial and temporal distributions possible. Emissions prepared for the 2006 platform benefit from several updates when compared to the former 2002 modelling platform.

The starting point for development of a modeling inventory is a database of emissions related data. The most reputable source of Canadian emission data is the National Emission Inventory databases (NPRI), maintained by Environment Canada. The database is summarized in the annual Canadian Comprehensive Criteria Air Contaminant Emission Inventory. Year 2006 was identified as the new base year for policy scenarios. Additional processing of the NPRI inventory for modeling platform affected industrial sources, on-road mobile emissions, and agriculture and fugitive dust emissions.

Another important step of modeling inventory development is the spatial allocation of emissions. Because Canadian area source emissions inventories are compiled on a provincial level, it is important that the physical location of emissions be determined as accurately as possible. Spatial surrogates were updated by using the latest socio-economic data from the 2006 Canadian census.

In addition to new surrogates for emission gridding, revisions were done for chemical speciation of emissions to model specific chemical mechanism. Several VOC and PM profiles were revised as well as the PM size disaggregation into twelve size bins.

In the next section a short description of the Canadian 2006 inventory is provided. Four major methodological changes appearing in this version of the modelling platform are then described. These are improved treatment of fugitive dust, revised VOC speciation profiles, revised PM speciation and size disaggregation and the new spatial allocation using 2006 census data from Statistic Canada and National Road Network (GEOBASE, 2009).

2. Summary of 2006 emission data

The Canadian 2006 comprehensive Criteria Air Contaminants (CAC) emissions inventory is used for the current 2006 modeling platform. This inventory includes reported air pollutant emissions for NO_x, VOC, NH₃, CO, SO₂, PM₁₀ and PM_{2.5} (see table 1).

Source	Description	CO	NH ₃	NOX	PM ₁₀	PM _{2.5}	SO ₂	VOC
Area	Incineration	2,534	75	283	13	8	1,725	668
	Industrial	176,139	1,573	27,132	58,120	22,522	14,466	51,979
	Miscellaneous	3,967	1,614		8,545	8,525		395,865
	Non-Industrial	723,525	1,954	86,927	112,056	110,993	44,109	155,521
	Opens Sources	22,371	499,450	3,469	1,670,454	259,243	887	309,668
	Forest fires	2,484,823	5,325	79,159	256,470	211,210	178	340,776
	On-road mobile	4,206,390	20,227	499,771	13,935	9,882	5,034	258,646
	Off-road mobile	2,758,024	736	731,019	59,258	56,251	102,502	313,568
Area Total		10,377,774	530,953	1,427,761	2,178,850	678,634	168,902	1,826,690
Point	Incineration	1,898	0	679	510	410	92	641
	Industrial	1,298,906	16,466	738,335	105,198	64,884	1,340,369	703,765
	Miscellaneous	7	0	37	172	60	0	14,936
	Non-Industrial	32,074	158	215,653	12,725	5,991	462,147	1,933
	Opens Sources	4,575	4,993	3,361	457	245	422	1,436
Point Total		1,337,460	21,617	958,066	119,063	71,590	1,803,029	722,711
Grand Total		11,715,233	552,570	2,385,826	2,297,913	750,224	1,971,931	2,549,402

Table 1: 2006 total anthropogenic emissions for Canada in metric tons

When compared to the 2002 version of the modeling platform, the 2006 platform include following changes:

- Better, updated CAC emission estimates,
- On-road mobile inventory based on a revised version of MOBILE6 for Canadian conditions, including biodiesel capability
 - Emissions by IM region instead of provincial total
 - Emissions by vehicle operation (EXH, EVAP)
 - Monthly emissions to account for temperature changes
- Most of the industries now in point source format with detail stack information, as opposed to area sources
- Detailed VOC speciation (ADOM-II, CB05, others) and temporal profiles for point sources, by sector
- Refined estimates of the fugitive dust emissions
- New VOC speciation for diesel vehicles
- Revised PM speciation and size disaggregation in 12 bins

- New spatial allocation with 2006 census data from Statistic Canada and National Road Network.
- Agricultural emissions from the comprehensive NAESI survey projected to year 2006 (Ayres et al., 2009; Bittman et al., 2008).

One limitation of the Canadian CAC inventory is the absence of SCC codes associated with individual point sources. This is addressed by using a cross-reference table associating Canadian activity sectors to SCC codes. The SMOKE tool can then be used, along with temporal and chemical ancillary data. This table was revised to better reflect the actual sector profiles in Canada.

3. Fugitive dust emissions

Estimates of fugitive dust emissions were implemented by using land-cover dependent transportable-fractions. Originally, the PM export fraction for fugitive dust sources was a constant factor of 25% across Canada. The new methodology allowed the factor to vary by landuse and source category in the inventory. Following is a brief description of the adjustments applied to determine the emissions transportation fraction.

Step 1 – Calculating the transportable fraction fields

The transportable fraction (TF) fields were calculated using land-use classes generated with the surface field generator GenPhysX. GenPhysX is a tool developed by Environment Canada to process geospatial databases and generate gridded data for Canadian meteorological and air quality models. It also has a module for biogenic emission generation. GenPhysX coverage is global, however some regions have higher resolution databases than others. Over North America, GenPhysX mainly uses the BELD3 vegetation database in addition to other databases at spatial resolution of 1 km. Table 2 shows the percent transportable fractions considered for different land use classes. The tool was applied over a continental domain at 45-km resolution. Figure 1 depicts the final transportable fraction for fugitive dust PM emissions.

Land use type	Transportable Fraction
Evergreen, deciduous and mixed forest	0%
Crops, mixed farming	75%
Dwarf trees, shrubs, tundra, grassland	75%
Wet land with plants	75%
Desert	100%
Ice caps and glaciers	100%
Inland water, Ocean	100%
Urban	50%

Table 2: Transportable Fractions for each land-use type

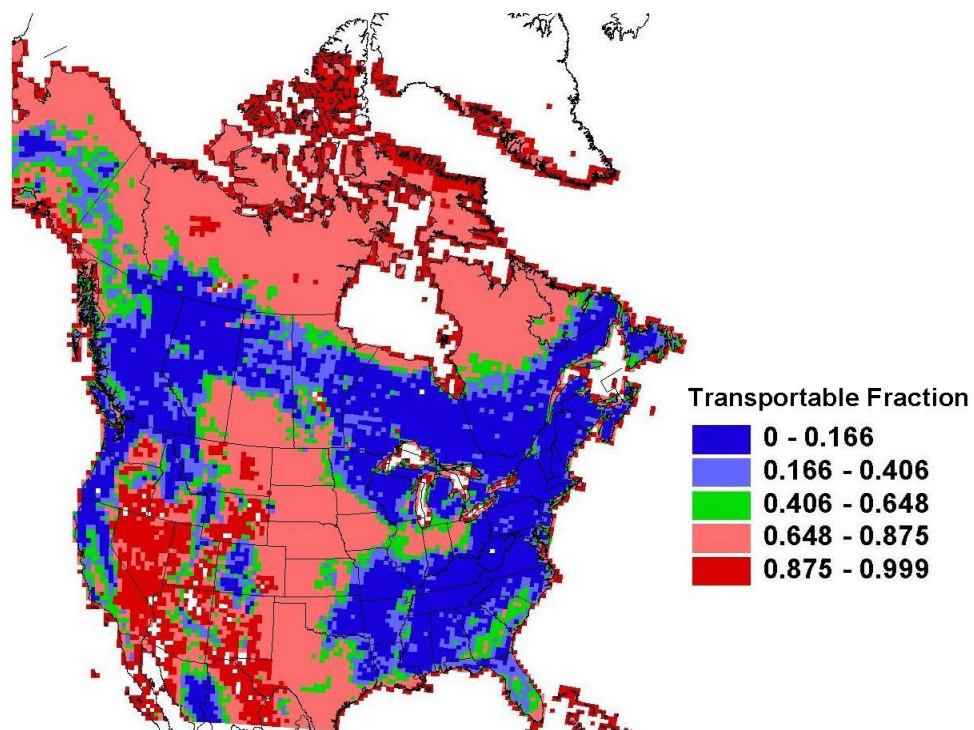


Figure 1: Transportable fraction over North American domain at 45-km resolution

Step 2 – Generating spatial surrogates

The Surrogate Tool (<http://www.ie.unc.edu/cemspd/projects/mims/spatial/>) was used to create a set of spatial surrogates. Output from the Surrogate Tool is a set of grid-based spatial surrogate ratio files to be used as input to the SMOKE processor (<http://www.smoke-model.org/>). Four spatial surrogates were created to distribute the fugitive dust emissions for different source emissions (see Figures 2a – 2d)

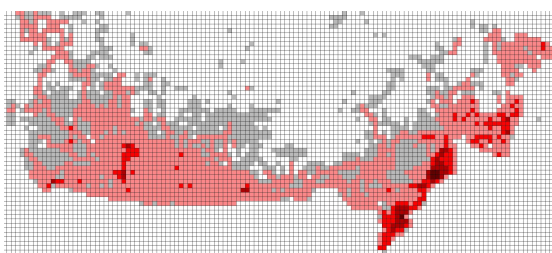


Figure 2 (a): Paved roads

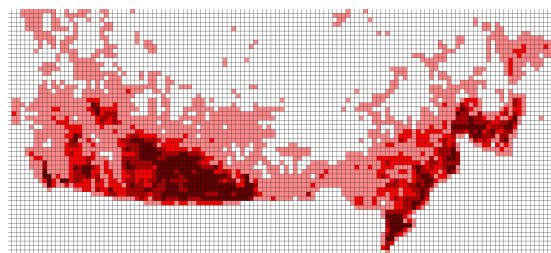


Figure 2 (b): Unpaved roads

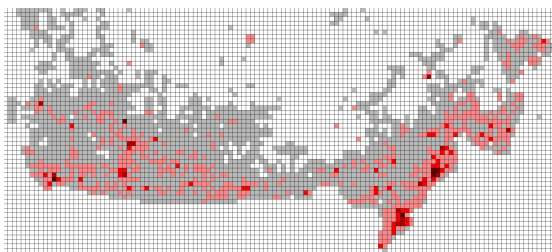


Figure 2 (c): Urban area

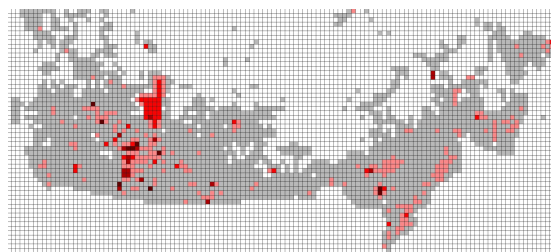


Figure 2 (d): Total mining

A cross reference table was applied to the fugitive dust sources to identify specific emission source category and the land-use class dependent transportable fractions (Table 3).

SCC description	SCC	Surrogate
Residential construction	2311010000	Urban area
Road construction	2311030000	Paved road
Heavy construction	2311020000	Total mining
Paved road	2294000000	Paved road
Unpaved road	2296000000	Unpaved road

Table 3: Cross reference table for fugitive dust emissions

Step 3 – Applying the transportable fraction to each spatial surrogate

A combination of surrogates and TF was generated. The new surrogate is calculated by intersecting each TF grid cell with the surrogate. The result is aggregated to the province level (see Table 4)

Province	Average TF	Urban area TF	Mining TF	Paved road TF	Unpaved road TF
AB	0.23	0.40	0.28	0.38	0.44
BC	0.24	0.27	0.08	0.19	0.12
MB	0.33	0.62	0.28	0.53	0.51
NB	0.21	0.30	0.22	0.18	0.09
NF	0.51	0.53	0.64	0.42	0.31
NS	0.51	0.27	0.26	0.33	0.24
ON	0.22	0.27	0.17	0.24	0.17
PEI	0.78	0.66	0.72	0.68	0.65
QC	0.33	0.26	0.23	0.20	0.10
SK	0.44	0.71	0.65	0.66	0.66

Table 4: Aggregation of the new transportable fractions at the provincial level for Canada

The PM transportable fraction estimates of road dust and construction sectors have shown reduction in QC, ON and BC provinces. However, they have increased in the prairies provinces, AB, MB and SK.

Step 4 – Scaling the emissions inventories with the new transportation fractions

The new combination of surrogates and TF factors were applied to the different fugitive dust emission inventories. Table 5 shows comparisons of TF factors using the original, 25% constant, and the new, land-use-dependent methods. The new transportation fraction for fugitive dust emissions showed very different results compared to the former methodology.

2006 PM _{2.5} fugitive dust	AB	SK	MB	NL	NS	PEI	NB	QC	BC	ON	Total
Paved roads	52%	164%	112%	68%	30%	170%	-30%	-20%	-23%	-5%	9%
Unpaved roads	75%	164%	106%	24%	-3%	161%	-65%	-59%	-53%	-32%	33%
Residential construction	62%	184%	148%	111%	7%	164%	22%	4%	8%	9%	45%
Heavy Construction	11%	161%	10%	155%	3%	189%	-11%	-8%	-66%	-31%	30%
Road Construction	52%	164%	112%	68%	30%	170%		-20%	-23%	-5%	45%
Total	50%	163%	100%	50%	14%	166%	-46%	-40%	-34%	-21%	28%

Table 5: Percentage difference in fugitive dust emissions calculated after using the old and the new TF method

3. New ADOM-II speciation input files for VOCs

Another major aspect of modeling inventory development is chemical speciation. This is the process of disaggregating inventory pollutants into individual chemical species components. VOCs are usually reported as lumped emissions in the CAC inventories. Speciation is done using the SMOKE emissions processor with user supplied chemical speciation profile. A chemical speciation profile tells the SMOKE processor how to fraction the input VOC emissions into individual air quality model mechanism species.

5 resolved single compounds	13 generic lumped compounds
1. Methane, 2. Ethane, 3. Ethene, 4. Isoprene, 5. Formaldehyde.	Single compounds - Propane as the representative species for low reactivity species propane, acetylene and benzene; - Toluene for all mono-substituted aromatics; - O-cresol for all cresols; - Aromatics for all xylenes and other di- and tri-substituted aromatics; - Acetaldehyde for acetaldehyde and all higher carbon number aldehydes; - Methy-ethyl-ketone for that compound and all higher carbon number ketones; - Methyl glyoxal for all glyoxals; - Peroxyacetylnitrate for PAN and all acyl nitrates; - Methyl nitrate and methyl peroxide representing all organic nitrates and organic peroxides.
	Lumped species with OH reaction rate constants derived from typical atmospheric levels of the observed species.
	- Higher alkanes; - Higher alkenes.
6 additional short lived organic intermediates	

Table 6: Descriptions of ADOM-II mechanism species

The regional air quality models at Environment Canada use the ADOM-II mechanism. The speciation file is based on the RADM file available with SMOKE. The VOC speciation was modified to reflect that of the ADOM-II mechanism, (Lurmann et al., 1986; Lurmann et al., 1984). Table 6 lists the VOCs considered in the ADOM-II mechanism.

New speciation profiles for diesel vehicle exhaust emissions using biodiesel fuels were developed using both the recently developed Canadian MOBILE6 output and laboratory measurements conducted within Environment Canada (Environment Canada, 2008). Figure 3 shows the gasoline, regular diesel (B00) and bio-diesel speciation profiles.

The bio-diesel speciation was developed for heavy diesel vehicles using two different percentage blends (5% and 20%).

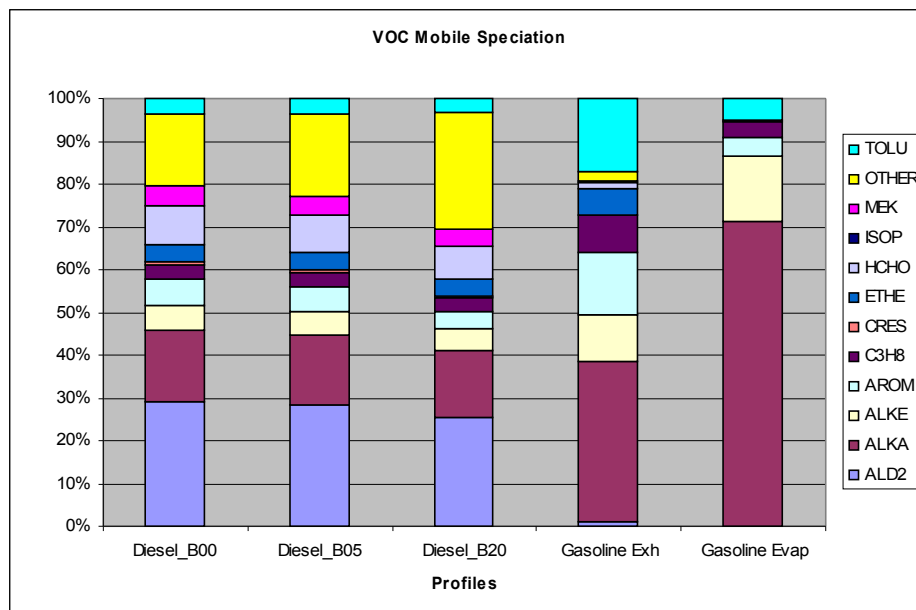


Figure 3: Gasoline and bio-diesel vehicle VOC emissions speciation profiles

3. PM speciation

PM Emissions for AURAMS air quality model (Gong et al., 2006) need to be speciated to chemical components as well as fractionated into different size bins. The raw emission inventory contains PM_{10} and $PM_{2.5}$ species, which is then further divided into source types by SCC codes. The PM species are sulfate, nitrates, soil dust, black carbon and organic carbon.

The tables below show how $PM_{2.5}$ is allocated in to size bins. Three categories are defined: one profile for mobile emissions, one for area emissions, and one for minor and major point emissions. The PM size distributions used for the four primary emissions streams are each a weighted average of measured PM size distributions for different source types presented in Figure 1 of Eldering and Cass (1996). Figure 4 shows the resulting 12-bin distributions.

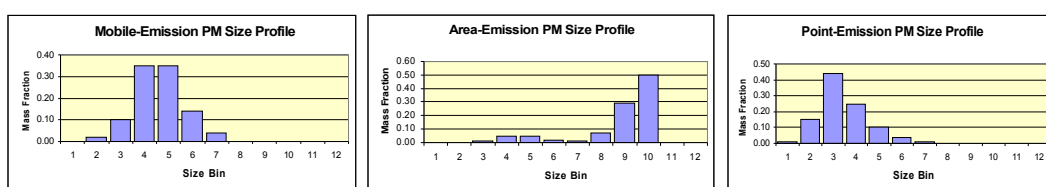


Figure 4: Particulate matter size distribution for mobile, area and point sources.

The combination of revised speciation by SCC codes and size disaggregation by three categories provides the best estimates of PM emissions used so far in Canadian air quality policy scenarios.

4. Spatial surrogates

A new set of spatial surrogates are made available for Canada. It is based on the 2006 census data from Statistic Canada. It contains 108 industries classes from North American Industry Classification System (NAICS) and an updated Canadian National Road Network (GEOBASE, 2009).

Spatial surrogates for mobile emissions require careful treatment. Since the Canadian mobile emission inventory is composed only by vehicle type while the surrogate data is based only on road class, it was necessary to develop spatial surrogates based on activity by vehicle types across all road classes.

These surrogates were developed as weighted population and roadway miles across all road classes. The weights are different for each vehicle type, and are based on the amount of VMT that vehicle travels on each of the road types. Surrogates were compiled for the seven vehicle types (LDGV, LDGT, HDGV, MC, LDDV, LDDT, and HDDV) by applying the US percentages of vehicle type - roadway type ratio to the four Canadian road classes.

	Highway, freeways	Primary road (arterials)	Secondary road (collectors)	Residential Street
VMT (%)	30%	42%	16%	13%

Figure 5: Average weight for all vehicle types based on VMT on each of the road types

5. Conclusion

The new 2006 Canadian emissions inventory for air quality model applications provides the following improvements:

- Updated emissions inventory data from the previous 2002
- More detailed on-road emissions inventory and revised chemical speciation
- Revised transport fraction calculation by land-use
- PM emissions speciation and size allocation by source type
- New set of surrogates based of 2006 census data from Statistics Canada

These improvements in the generation of Canadian emissions modelling files allow greater flexibility in the design of air quality modelling scenarios.

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