2006 ANNUAL OPERATIONAL EVALUATION OF THE ENVIRONMENT CANADA AIR QUALITY MODELLING SYSTEM

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*1. Introduction

Environment Canada is establishing an air quality policy modelling platform for simulation year 2006. The objective is to adopt the latest air quality science and model technology to build sets of tools, upon which, sound advice can be given to policy managers. The results from the platform can be used for assessments of air quality regulations and proposals across different regions and cities in North America. This work is built upon a previous annual simulation for 2002 (Moran et al., 2008).

The development of the 2006 modelling platform includes many aspects of data process before and after the actual chemical transport simulation. It encompasses setting appropriate model domains, establishing annual meteorology and emission data, conducting model validation against surface measurements, and post-processing of model results for health and environmental benefit assessments.

The new platform enhances from a previous 2002 annual simulation in many aspect, such as, domain nesting capabilities, updated emissions processing, flexibility in emission scenario selection, dynamic lateral ozone boundary conditions, and an integrated model evaluation system.

In this presentation, we will provide an overview of the new 2006 modelling platform. We first outline the general model configuration, and simulation setup, followed by descriptions of a new integrated database verification system. Finally, we will present preliminary model evaluation results for ground level O_3, $PM_{2.5}$, NO_2, and speciated $PM_{2.5}$ comparing with routine surface measurements.

2. Modelling Platform

Figure 1 shows the schematic of the AURAMS modelling system in the platform. The system consists of three main components: the GEM prognostic meteorological driver, the SMOKE emissions processing system, and the core, off-line, regional chemical transport model, AURAMS CTM.

Figure 2 shows the simulation domains for the platform. Additional descriptions of the individual modelling components are provided in the following subsections.

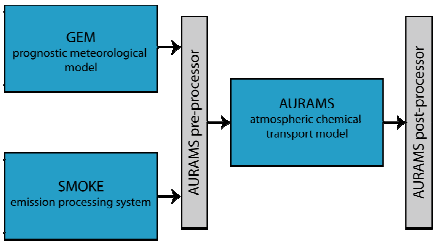

Figure 1. Schematic of the AURAMS modelling system.

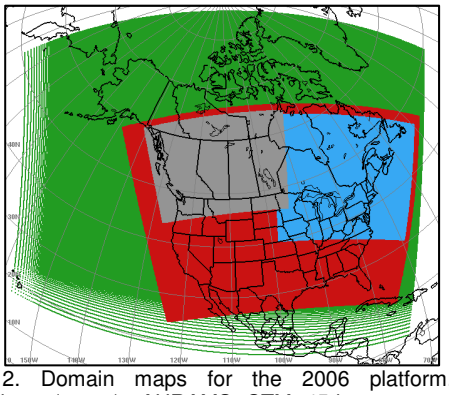

Figure 2. Domain maps for the 2006 platform. GEM meteorology (green), AURAMS CTM 45-km parent domain (red) and two 22.5-km inner nested domains (blue and gray).

2.1 Meteorology

The GEM meteorological model is Environment Canada's integrated weather forecasting system for both short- and medium-range weather forecasts (Côté et al., 1998). For the platform, GEM version 3.3.2 with physics version 4.7.2 was applied on a variable horizontal domain with 575 x 641 points on a rotated latitude-longitude projection (Fig. 2). The domain has a core 432 x 565 uniform regional grid over North America with horizontal resolution of ~15-km.

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Vertically, there are 58 hybrid levels that increase monotonically with height from surface to ~10 hPa.

For the annual simulation, GEM was run in series of 30-hr segments with each segment initialized from analyses fields. The first 6 hours of each segment were discarded as spin-up. Model results from GEM were interpolated for input into AURAMS CTM.

The GEM model performance, as objective scores, against surface (pressure, temperature, precipitation and dew point) and upper air (geopotential height, temperature, wind and dew point) comparisons were analyzed for the 2006 annual simulation. Results showed that the model performed adequately compare to operational forecast system. For more information on GEM setup and meteorological evaluation please refer to Pavlovic et al. (2009).

2.2 Emissions

Hourly anthropogenic emissions for the platform were prepared using the SMOKE (v2.4) system. Input emissions inventory include: 2006 Canadian Criteria Air Contaminants emission inventory (CAC version 2), the 2005 United States National Emission Inventory (NEI version 5), and 1999 Mexican inventory.

Canadian CAC inventory is based on the National Pollutant Release Inventory (NPRI) of Environment Canada (http://www.ec.gc.ca/inrp-npri). Emissions for United States and Mexican were obtained from the EPA emissions clearinghouse (http://www.epa.gov/ttn/chief/emch).

There are several changes in the 2006 Canadian emissions inventory compare to the previous 2002 annual simulation. Some highlights are:

- New spatial allocation with 2006 census data
- Revised PM speciation profiles that vary by source category
- 12-bin PM size disaggregation by source
- New point source VOC speciation and temporal profiles by emission sectors
- New monthly mobile source emissions by vehicle inspection/maintenance (I/M) regions; emissions by evaporative and exhaust fractions instead of total VOC
- New fugitive dust emissions with land-cover dependent transportable fractions.
- New agriculture NH_3 emissions based on the National Agri-Environmental Standards Initiative (NAESI) survey (Ayres et al., 2008)

The emissions data not only updated the quantitative estimates, but also improved upon their spatiotemporal representation and chemical characterization. For additional information please refer to Sassi et al. (2010).

Biogenic emissions for the annual simulation were estimated online by AURAMS CTM using BEIS v3.09 algorithms. Emissions were adjusted with hourly surface temperature and solar fluxes.

2.3 AURAMS CTM

AURAMS CTM is a multi-pollutant off-line AQ model that describes the formation of ozone, PM and acid depositions. PM distribution in the model is represented using 12 bins ranging from 0.01 to 41 μm in diameter. PM consists of internally mixed chemical components: sulfate, nitrate, ammonium, elemental carbon, primary organic aerosol, secondary organic aerosol, crustal material, sea salt and particle-bound water.

Gas phase chemistry is modelled using a modified version of the ADOM-II (Acid Deposition and Oxidation Model) chemical mechanism. Aerosol dynamics and aqueous-phase processes include size-resolved nucleation, condensation, coagulation, activation, and sedimentation (Gong et al., 2007). Inorganic heterogeneous chemistry is represented by the HETV scheme with ISSORPIA, and a two-product secondary organic aerosol scheme following Jiang (2003).

Ozone boundary conditions for the parent domain were derived from observational with dynamic tropopause height adjustments (Makar et al., 2010; Samaali et al., 2009).

Figure 2 depicts the AURAMS CTM domains in polar stereographic projection. The parent domain has 45-km grid spacing at 60°N, with 143x107 grids. Two nested domains at 22.5-km resolution are defined for eastern (145x123) and western (124x93) Canada. The nested domains were chosen to cover major portions of Canada. Vertically, all three domains have 28 terrain-following levels from surface to 29 km.

The annual simulation was carried out concurrently in three segments: (1) 2005-12-10 to 2006-06-01, (2) 2006-05-01 to 2006-10-01, and (3) 2006-06-01 to 2006-12-31. The first 20 days in the first segment, and the one-month overlaps in the last two segments were discarded as model spin-up. Results from the three segments were stitched together for a complete, annual simulation.

3. Verification Database and Measurement Data

Major effort was invested to develop an integrated database system for model verification. The advantages of a model evaluation database have been described and demonstrated previously (CMAS AMET, 2008). Additional factors considered were information traceability, results reproducibility, and ease of automation in an operational setting. A similar evaluation database is being adopted for Environment Canada's GEM-MACH real-time air quality forecast system (Ménard, et al., 2010).

The verification database is based on the open source PostgresSQL relational database with PostGIS geospatial extension. A unique feature of the system is the ability to store and process geospatial information relevant to model analyses.

The additional geospatial capabilities add new dimensions to how we examine model performance. For example, we can easily group and select measurement stations base on spatial information such as land use and land cover, population density, distance from highways and other spatial topological relations. Model performance results can be easily exported to widely-supported file formats such as csv, shapefiles, KML files. Visualization is possible with software such as Google Earth and QuantumGIS or by direct connection to the database server.

For the 2006 platform, verification was conducted by comparing model results with routine, high resolution surface measurements within the model domain. Model results were paired with available surface observations spatiotemporally and by chemical species.

Measurements were compiled from two national networks: the Canada NAPS (http://www.ec.gc.ca/rnspa-naps) and the US EPA AQS (http://www.epa.gov/ttn/airs/airsaqs/). Currently, only hourly measurements are included in the database, and only O_3, $PM_{2.5}$, and NO_2 are presented here. Standard model performance statistics by different temporal and spatial measures were queried directly from the database.

Additional evaluations for speciated $PM_{2.5}$ were carried out with NAPS measurements outside of the verification database. Table 1 shows the total number of station and data points considered.

Table 1: Number of stations and data considered in the model evaluation

	USA AQS		Canada NAPS	
	sites	datapoints	sites	datapoints
Hourly O_3	1147	7,281,543	194	1,560,483
Hourly $PM_{2.5}$	520	4,064,250	173	1,283,799
Hourly NO_2	399	2,962,403	136	998,496
24hr PNO3			35	1,739
24hr PSO4			32	1,923
24hr PNH4			32	1,868
24hr EC2.5			12	995
24hr OC2.5			12	899

4. Model Performance Evaluation

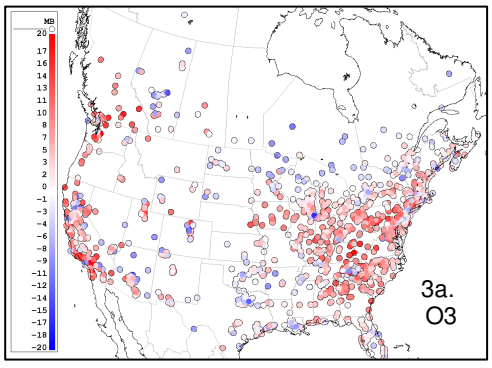
Results from the parent domain were compared against surface measurements from both the Canadian NAPS and US AQS networks, while results from the inner domains were compared only with the Canadian NAPS network. A final section demonstrates evaluation by population density with results from the inner domains.

4.1. Coarse Domain O_3, NO_2 and $PM_{2.5}$

Hourly model results were compared with surface measurements by site and for all available measurement data. Results were averaged across all sites within a network, and temporally by season and year.

Figure 3a, 3b, and 3c show the spatial distribution of measurement stations and the annual averaged mean bias for O_3, NO_2 and $PM_{2.5}$, respectively.

Generally, there are higher O_3 biases for stations in eastern US, west coast US, and in the province of British Columbia, Canada. Low ozone biases are observed for stations in eastern Canada, and central US. For NO_2 and $PM_{2.5}$, the model mostly under-predicted, except for few selected urban areas where the model showed higher biases.



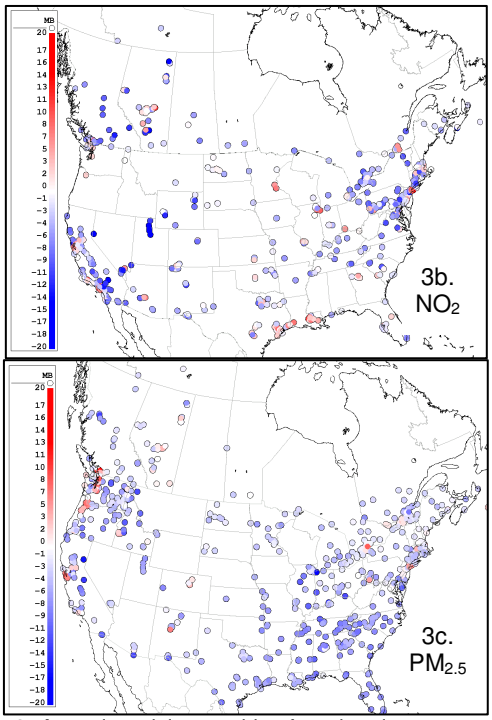


Figure 3: Annual model mean bias from hourly measurements for O_3 (ppbv), NO_2 (ppbv) and $PM_{2.5}$ ($\mu g/m^3$).

Table 2, 3 and 4 show the averaged seasonal and annual concentrations and performance statistics for O_3, NO_2 and $PM_{2.5}$, respectively. Model performances are slightly different between Canada and the US, and vary by seasons. The model showed better correlation for gaseous species, O_3 and NO_2, than $PM_{2.5}$. Annual and seasonal concentrations are generally higher in the US, and the model captured the differences appropriately.

Annually, there are positive biases for O_3 and negative biases for NO_2 and $PM_{2.5}$. Normalized mean error is much smaller for O_3 than NO_2 and $PM_{2.5}$. Seasonally, the model under-predicted low winter ozone, and over-predicted high summer ozone. In both US and Canada, the model had highest O_3 error and positive bias in the fall and lowest in spring. The model also captured the high winter and low summer NO_2; as well as the high $PM_{2.5}$ in both summer and fall.

Table 2: Model performance statistics for O_3 (ppbv); modeled mean, observed mean, normalized mean bias (NMB), normalized mean error (NME), and correlation coefficient (R).

CANADA	DJF	MAM	JJA	SON	YEAR
mod. mean	22	32	26	19	25
obs. mean	18	29	30	23	25
NMB	-16%	-9%	16%	24%	3%
NME	40%	32%	37%	47%	38%
R	0.51	0.48	0.66	0.51	0.57
USA					
mod. mean	23	36	36	26	32
obs. mean	22	37	42	31	35
NMB	-2%	3%	15%	19%	10%
NME	40%	29%	35%	41%	35%
R	0.57	0.63	0.68	0.65	0.68

Table 3: Model performance statistics for NO_2 (ppbv)

CANADA	DJF	MAM	JJA	SON	YEAR
mod. mean	14	11	9	11	11
obs. mean	9	8	7	9	8
NMB	-35%	-32%	-20%	-20%	-28%
NME	57%	64%	66%	61%	62%
R	0.48	0.48	0.47	0.49	0.48
USA					
mod. mean	16	11	10	13	12
obs. mean	12	9	9	11	10
NMB	-24%	-18%	-6%	-15%	-16%
NME	51%	62%	69%	58%	59%
R	0.59	0.56	0.51	0.58	0.56

Table 4: Model performance statistics for $PM_{2.5}$ ($\mu g/m^3$)

CANADA	DJF	MAM	JJA	SON	YEAR
mod. mean	7	6	8	7	7
obs. mean	6	6	7	7	6
NMB	-14%	-8%	-16%	9%	-8%
NME	77%	73%	65%	81%	73%
R	0.29	0.13	0.35	0.33	0.2
USA					
mod. mean	11	10	13	11	11
obs. mean	7	7	9	9	8
NMB	-34%	-35%	-31%	-21%	-31%
NME	63%	63%	57%	62%	61%
R	0.39	0.34	0.4	0.35	0.38

4.2. Inner Domain Speciated $PM_{2.5}$

$PM_{2.5}$ for sulfate (PSO4), nitrates (PNO3), ammonium (PNH4), elemental carbon (PEC), and organic carbon (POC) were compared with 24-hr averaged filter measurements from NAPS. Most measurement stations are located in or near urban centers south of Canada (Fig. 4).

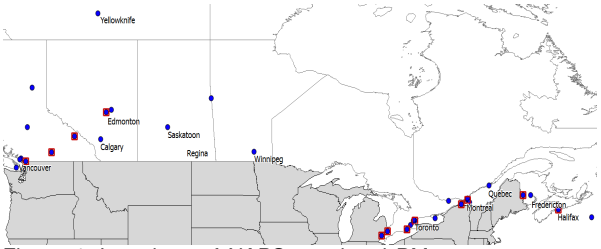


Figure 4: Locations of NAPS speciated $PM_{2.5}$ measurements. Red square indicates sites with PEC/POC measurements.

Scatter plots of daily measurements for each of the $PM_{2.5}$ component species (Fig. 5) showed the model performed better for PNH4 and PSO4. There are consistent low bias for POC, and high bias for PNO3 in the summer.

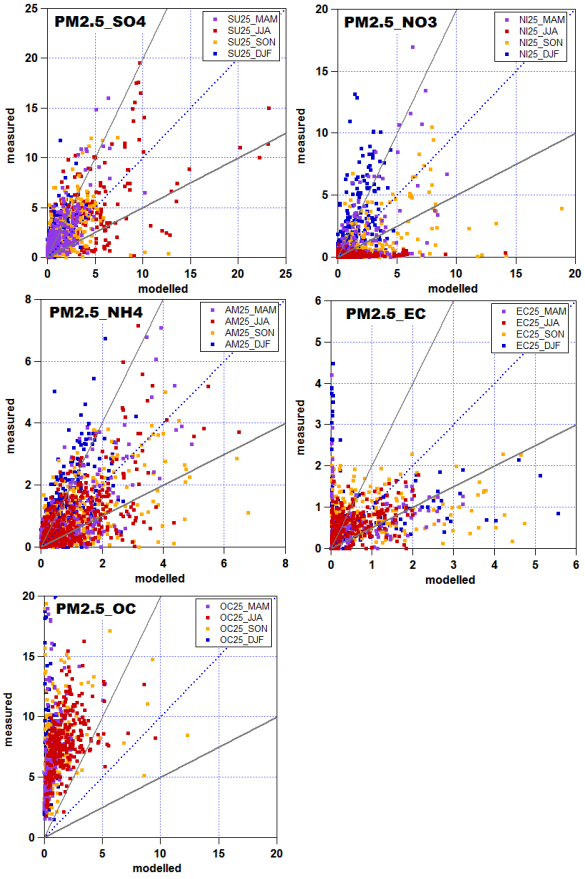


Figure 5: Scattered plots of 24-hour speciatedPM2.5, with 1:1 and 1:2 lines. Season is indicated by colour.

Table 5 to 9 show the detailed seasonal and annual model performance statistics averaged across all stations. AURAMS captured the temporal correlation very well for PNH4 and PSO4, but less so for PNO3, POC, and PEC.

The model represented annual mean concentrations adequately for all species except POC. The model significantly underestimates the annual POC by -86%. This is likely due to under-representation of biogenic secondary organic aerosols, and no semi-volatile species. An updated version of AURAMS has been shown to improve POC results (Stroud et al., 2010).

Seasonal correlation was higher for PNH4 and PSO4, but low for PNO3 and rather poor for PEC and POC. There are consistent positive biases for PEC and negative biases for PSO4 and POC in all seasons.

PNO3 showed significant high positive bias throughout spring and fall, and negative bias in the winter. The positive bias is likely due to known measurement artifacts (sample loss by volatilization) in the NAPS network as reported by (Brook and Dann, 1999).

Table 5: Model performance statistics for PSO4 (µg/m^3)

	DJF	MAM	JJA	SON	YEAR
mod. mean	0.8	1.0	2.2	1.3	1.4
obs. mean	1.7	1.8	2.4	1.8	1.9
NMB	-56%	-44%	-10%	-28%	-30%
NME	63%	56%	59%	55%	58%
R	0.62	0.74	0.69	0.55	0.65

Table 6: Model performance statistics for PNO3 (µg/m^3)

	DJF	MAM	JJA	SON	YEAR
mod. mean	1.0	1.3	0.7	1.5	1.1
obs. mean	1.6	0.8	0.1	0.7	0.8
NMB	-40%	52%	457%	126%	43%
NME	67%	125%	511%	158%	122%
R	0.63	0.55	0.23	0.54	0.43

Table 7: Model performance statistics for PNH4 (µg/m^3)

	DJF	MAM	JJA	SON	YEAR
mod. mean	0.6	0.8	0.9	0.9	0.8
obs. mean	1.0	0.8	0.8	0.7	0.8
NMB	-38%	-1%	17%	25%	0%
NME	57%	61%	66%	67%	62%
R	0.70	0.73	0.68	0.64	0.64

Table 8: Model performance statistics for PEC (µg/m^3)

	DJF	MAM	JJA	SON	YEAR
mod. mean	0.7	0.6	0.5	0.8	0.7
obs. mean	0.8	0.6	0.6	0.7	0.7
NMB	22%	32%	14%	59%	33%
NME	99%	100%	90%	138%	109%
R	0.14	0.24	0.48	0.19	0.22

Table 9: Model performance statistics for POC (µg/m^3)

	DJF	MAM	JJA	SON	YEAR
mod. mean	2.1	1.9	2.6	2.4	2.3
obs. mean	7.6	6.8	7.9	7.2	7.4
NMB	-73%	-73%	-67%	-67%	-69%
NME	75%	73%	67%	70%	71%
R	0.10	0.28	0.47	0.37	0.26

4.3. Evaluation by Geospatial Attribute

A 2006 Canada census data for population density by dissemination areas was loaded into the model evaluation database. Using this information, we can easily select and filter measurement stations based on ranges of population density.

Figure 6 shows the NAPS measurement stations by four levels of population density. They were selected to represent: urban (>4000 people/km^2), suburban (4000-1000 people/km^2), semirural (1000-100 people/km^2) and rural (< 100 people/km^2) areas.

Using these criteria, we calculated the general model performance statistics for the selected stations in each category (Fig 7). The results showed a clear trend of higher surface ozone from rural to urban stations, and that the model was

able to capture this, albeit with higher negative bias in urban area, and lower errors in other areas.

The concentration trend was reversed for $PM_{2.5}$ and NO_2; higher concentrations were observed in urban areas, and decrease with rural settings. Model errors also decreased with concentrations. There are relatively higher $PM_{2.5}$ and NO_2 biases in urban stations than other environments.

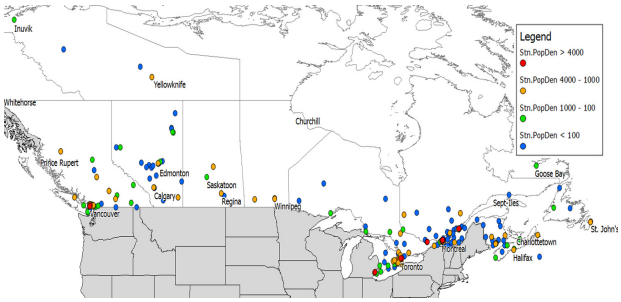


Figure 6: NAPS measurement sites with different levels of population density.

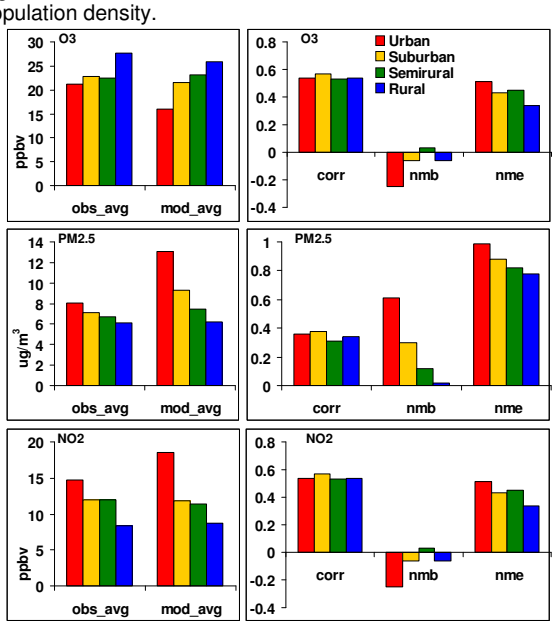


Figure 7: Annual average hourly measured and modelled O_3 (top), $PM_{2.5}$ (middle) and NO_2 (bottom) concentrations and their model performance statistics by population density levels.

5. REFERENCES

Ayres, J., Bittman, S., Sheppard, S., and Girdhar, S., Sources of ammonia emissions. In: C. Lillyman and K. Buset, Editors, 2008 Canadian Atmospheric Assessment of Agricultural Ammonia, pp. 112–130. National Agri-Environmental Standards Technical Series Report No. 4-1.

Brook, J.R. Dann, T.F., Contribution of nitrate and carbonaceous species to PM2.5 observed in Canadian cities, Journal of The Air & Waste Management Association Volume: 49 Issue: 2 (1999-01-01) p. 193-199.

CMAS, Atmospheric Model Evaluation Tool (AMET) User's Guide, 2008, available online: http://www.cmascenter.org/help/model_docs/amet/1.1/AMET_Users_Guide_V1.1.pdf.

Côté, J., J.-G. Desmarais, S. Gravel, A. Méthot , A. Patoine, M. Roch and A. Staniforth, 1998, Mon. Wea. Rev., 126, 1373-1395.

Gong, S.L., L.A. Barrie, J.-P. Blanchet, K. von Salzen, U. Lohmann, G. Lesins, L. Spacek, L.M. Zhang, E. Girard, H. Lin, R. Leaitch, H. Leighton, P. Chylek, and P. Huang, 2003: Canadian Aerosol Module: A size segregated simulation of atmospheric aerosol processes for climate and air quality models: Part 1. Module development. J. Geophys. Res., 108(D1), 2007, doi:10.1029/2001JD002002, 16 pp.

Jiang, W., Instantaneous secondary organic aerosol yields and their comparison with overall aerosol yields for aromatic and biogenic hydrocarbons. Atmos Environ. 2003, 37, 5439–5444.

Makar, P.A., V.S. Bouchet, and A. Nenes, Inorganic chemistry calculations using HETV˜ a vectorized solver for the SO42- NO3˜-NH4+ system based on the ISORROPIA algorithms. Atmos. Environ., 2003, 37, 2279-2294.

Makar, P.A, W. Gong, C. Mooney, J. Zhang, D. Davignon, M. Samaali, M.D. Moran, H. He, D. Tarasick, D. Sills, J. Chen, Dynamic adjustment of climatological ozone boundary conditions for air-quality forecasts, Atmospheric Chemistry and Physics, 2010, 10, 8997–9015.

Ménard S, R. Pavlovic, M.D. Moran, P-.A. Beaulieu, S. Gilbert, J. Chen, P.A. Makar, and G. Morneau, GEM-MACH15 Operational Air Quality Forecast Model: An Evaluation of the First Year's Performance, to be presented at the 2010 International Workshop on Air Quality Forecasting Research, Quebec City, Canada.

Moran, M. D., Q. Zheng, M. Samaali, J. Narayan, R. Pavlovic, S. Cousineau, V. S. Bouchet, M. Sassi, P. A. Maker, W. Gong, S. Gong, C. Stroud and A. Duhamel, 2008, Comprehensive surface-based performance evaluation of a size- and composition-resolved regional particulate-matter model for a one-year simulation, Air Pollution Modelling and Its Application XIX, 2008, 4, 434-442.

Pavlovic, R., J. Chen, S. Cousineau, L-P. Crevier, Davignon, D., A. Duhamel, S. Gilbert, J. Racine, M. Samaali, M. Sassi, The impact of meteorological variability on the modelling of air quality scenarios, 2009, 8th Annual CMAS Conference, Chapel Hill, , NC, USA.

Samaali, M., Moran, M. D., Bouchet, V. S., Pavlovic, R., Cousineau, S., and Sassi, M.: On the influence of chemical initial and boundary conditions on annual regional air quality model simulations for North America, Atmos. Environ., 43(32), 4873–4885, 2009.

Sassi, M., J. Chen, S. Cousineau, L-P. Crevier, A. Duhamel, S. Gilbert, R. Pavlovic, J. Racine, M. Samaali, M. Sassi, Evaluation of the 2006 Canadian air quality modelling platform for policy scenarios, 2010, EPA Emissions Inventory Conference, San Antonio, TX, USA.

Stroud C., P. Makar, M. Moran, W. Gong, S. Gong, J. Zhang, K, Hayden, C, Mihele, J. Brook, J, Abbatt and J. Slowick, Impact of Model Grid Spacing on Regional Air Quality Predictions of Organic Aerosol, 2010, 9th CMAS conference Chapel Hill, NC, USA.