A COMPARATIVE PERFORMANCE EVALUATION OF THE AURAMS AND CMAQ AIR QUALITY MODELLING SYSTEMS

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1. INTRODUCTION

A comparative performance evaluation has been conducted for the AURAMS (A Unified Regional Air-quality Modelling System) and CMAQ air-quality (AQ) modelling systems, developed by Environment Canada (EC) and the U.S. Environmental Protection Agency (EPA), respectively. This study was unique in that many aspects of the AURAMS and CMAQ simulations were purposefully "aligned" in order to reduce some of the common sources of differences between the models.

The two AQ models were run for a 696-hour period starting at 0100 UTC 1 July 2002 and ending at 0000 UTC 30 July 2002 over a continental North American domain. Each model used 42-km horizontal grid spacing and the model domains cover approximately the same land area. Emission files were generated from the same Canadian, U.S., and Mexican raw emissions inventories and the same biogenic emissions model (BEISv3.09). The raw emissions were processed using the SMOKE (Sparse Matrix Operator Kernel Emissions) emissions processing system, developed by the Carolina Environmental Program (CEP). Meteorological fields generated by the EC GEM (Global Environmental Multiscale) meteorological model were used as input to both the emissions processor and the two chemical transport models (CTMs).

Both AQ models were run in their "native" states to provide a baseline comparison of the two sets of modelling results. Despite the best-possible alignment of the two models, there still exist many differences between the "native" states of the models. Some key differences related to the model setup and operation include differences in "native" map projections, vertical coordinate systems, gas phase chemical mechanisms, aerosol representations, meteorological pre-processors, and emissions processing methods. In addition, there are also numerous differences in detailed scientific processes embedded in the models. All of these differences contribute to each models' behaviour and performance.

Our methodology, however, precludes or greatly reduces the impacts of the other components of the system aside from the CTMs themselves, and gives us more confidence that the observed differences result from the AQ models, as opposed to the meteorological and/or emissions inputs to those models.

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2. MODELLING SYSTEMS DESCRIPTION

2.1. The AURAMS Modelling System

AURAMS is an AQ modelling system with size- and composition-resolved particulate matter (PM) representation. The AURAMS modelling system consists of three major components: an emissions processor; a meteorological driver; and a CTM (Gong et al., 2006). The AURAMS system also contains pre-processors that calculate biogenic emissions using the Biogenic Emissions Inventory System v3.09 (BEISv3.09) and transform emissions and meteorological data into a form useable by the CTM.

Emissions are processed using the SMOKE processor/model (CEP, 2005) and converted from I/O API format to Recherche en Prévision Numérique (RPN) standard format (Chartier, 1995) for use in AURAMS.

Predicted meteorological fields from the GEM model (Côté et al., 1998a,b) stored at every AURAMS advection time step (15 min) are used to drive the AURAMS CTM after transformation by the AURAMS meteorological pre-processor (Cousineau, 2003).

AURAMS was designed to be a "one atmosphere" or "unified" model in order to address a variety of interconnected tropospheric air pollution problems ranging from ground-level ozone (O_3) to PM to acid rain. As such, AURAMS treats gas-phase species and PM formation and evolution with time, as well as their interactions through gaseous, aqueous, and heterogeneous reactions and physical processes.

Nine chemical components, are considered to contribute to PM composition: sulphate (SU), nitrate (NI), ammonium (AM), black carbon (EC), primary organic aerosol (PC), secondary organic aerosol (OC), crustal material (CM), sea salt (SE), and particle-bound water (WA). AURAMS represents the PM size distribution using 12 size bins, ranging from 0.01 to 40.96 µm in diameter, with the PM chemical components assumed to be internally mixed in each size bin.

The gas phase chemistry is modelled using a modified version of the ADOM-II (Acid Deposition and Oxidant Model) chemical mechanism (Stockwell and Lurmann, 1989; Lurmann et al., 1986). Although AURAMS includes sea-salt emissions, sea-salt chemistry is not considered. Organic aerosol chemistry is modelled using the approach of Odum et al. (1996), and Jiang (2003). Inorganic aerosol calculations are performed using multiple chemical domain activity coefficient iterations (Makar et al, 2003). Aqueous-phase processes in AURAMS include size-resolved aerosol activation, aqueous-phase chemistry and wet deposition (Gong et al., 2006).

For this comparative modelling study, AURAMS v1.3.1b was run with 12-hour restarts for the complete 696-hour simulation period.

2.2. The CMAQ Modelling System

Similar to the AURAMS modelling system, the CMAQ modelling system (Byun and Ching, 1999) consists of three major components: an emissions processing system; a meteorological driver; and a CTM. The CMAQ modelling system also contains three other pre-processors for initial conditions, boundary conditions, and photolysis rates.

As with AURAMS, emissions files are generated by the SMOKE processor/model. In contrast to AURAMS, the emissions files are used directly by CMAQ without file format conversion.

GEM was used as the meteorological driver in CMAQ in order to align with the AURAMS modelling system. The GEM meteorological fields are processed by the GEM Meteorology Chemistry Interface Program (GEM-MCIP) (Yin, 2004), developed in-house at the National Research Council of Canada (NRC), to transform the GEM fields into a form useable by SMOKE and CMAQ.

In CMAQ, particle size distributions are represented as a superposition of three log-normal sub-distributions or modes: Aitken or i-mode; accumulation or j-mode; and coarse or c-mode (Binkowski and Roselle, 2003). The PM concentrations generated by CMAQ cover the complete log-normal distributions and are not directly comparable with size-resolved measurement data. In this study, the PMx postprocessor, developed in-house at NRC (Jiang and Yin, 2001; Jiang et al., 2006b), is used to calculate particle size distribution parameters and PM concentrations within required particle size ranges. Calculations are done on the basis of classical aerodynamic diameter (Jiang et al., 2006a) to facilitate comparison with field measurement data (Jiang et al., 2006b).

CMAQ considers 12 species to contribute to PM composition: sulphate (ASO4), nitrate (ANO3), ammonium (ANH4), primary anthropogenic organics (AORGPA), secondary anthropogenic organics (AORGA), secondary biogenic organics (AORGB), elemental carbon (AEC), other fine PM mass (A25), aerosol water (AH2O), soil derived dust (ASOIL), other coarse mass (ACORS), and sea-salt (ACL and ANA).

CMAQ v4.6 was run for the 696-hour simulation period using 24-hour restarts, the SAPRC-99 chemical mechanism (Carter, 2000a,b), and the AERO4 aerosol module.

A more detailed description of the AURAMS and CMAQ AQ modelling systems, including CTM science components and 3-D grid definition, is available in Smyth et al. (2007).

2.3. Comparison of the AURAMS and CMAQ Grids

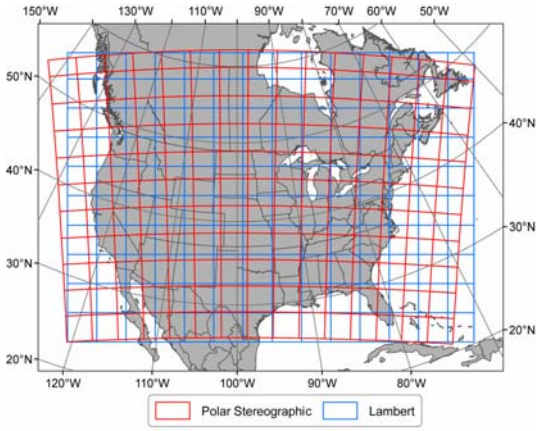

Fig. 1. The AURAMS polar stereographic domain and CMAQ Lambert conformal conic domain, displayed on the Lambert projection map.

The AURAMS modelling system uses a polar stereographic (PS) map projection as the basis for defining the horizontal grid. For this study, the Environment Canada “cont42” PS domain was adopted, consisting of 150 columns and 106 rows, with 42-km grid resolution.

The CMAQ modelling system uses a Lambert conformal conic (LCC) map projection in its “native” state. For this study, the LCC domain was

defined to "match" the AURAMS PS domain. The developed LCC grid consists of 139 columns and 99 rows with 42-km grid resolution and covers approximately the same geographical area as the PS grid as shown in Fig. 1.

3. COMPARISON OF METEOROLOGICAL AND EMISSIONS INPUTS

Evaluation of the processed meteorological fields input into each AQ modelling system showed minor differences in surface temperature, pressure, and specific humidity with normalized mean errors (NME) ranging from 0.25% to 3.8% when calculated over all over-lapping surface grid cells and the entire simulation period. These differences result from differences in the meteorological pre-processors and differences in map projections, which affect grid alignment.

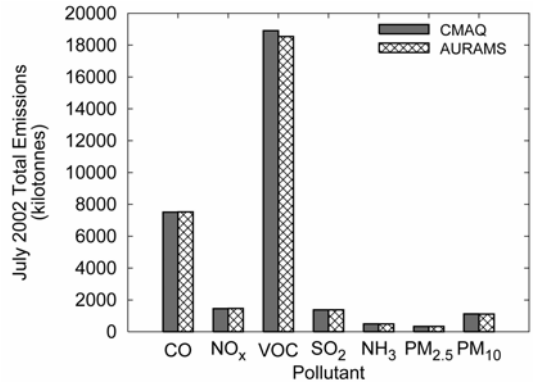

Fig. 2. Comparison of AURAMS and CMAQ anthropogenic and biogenic emissions totalled over the simulation period and respective domains.

Fig. 2 shows the comparison AURAMS and CMAQ anthropogenic and biogenic emissions totalled over each respective domain, all vertical levels, and the entire simulation period. The total emissions are similar for all criteria contaminants. More detailed analysis showed that total anthropogenic emissions were virtually identical for the two modelling systems, while there were slight differences in biogenic emissions of NO and VOCs. Since only minor variations in input temperature and pressure were present and identical biogenic emission factors were used, it is likely that the differences in biogenic emissions result from differences in solar radiation, BELD3 land-use data, and/or the implementation of the BEISv3.09 model in the modelling systems.

Analysis of temporal and spatial emission patterns (not shown) suggested that differences in input emissions can be caused by differences in speciation profiles, differences in processing major-point sources, and the differences in "true" grid cell size. The PS domain uses 15 900 42-km grid cells to cover approximately the same land area as the LCC domain which uses 13 761 42-km grid cells, meaning that the average PS grid cells are slightly smaller in "true" size than average LCC grid cells. Because of this, an average LCC grid cell contains more emission sources than a corresponding average PS grid cell.

4. COMPARISON OF O_3 PERFORMANCE

Performance statistics for AURAMS- and CMAQ-modelled ground-level ozone (O_3) in comparison with measurement data are summarized in Table 1. Hourly measurement data was taken from the National Air Pollution Surveillance (NAPS) and Air Quality Service (AQS) networks, administered by EC and the U.S. EPA, respectively.

Both models over-predicted O_3 concentrations. AURAMS had a lower bias than CMAQ with a normalized mean bias (NMB) of 17.9% versus 44.5% for CMAQ. In terms of error, the models' performance was more similar, with AURAMS performing slightly better with a NME of 45.6% versus 52.8% for CMAQ. In terms of correlation, the AURAMS r^2 of 0.39 was slightly lower than the CMAQ value of 0.44.

Table 1. AURAMS and CMAQ O_3 and daily peak O_3 statistics for 3-30 July 2002.

performance statistics	O_3 (ppb)		daily peak O_3 (ppb)	
	AURAMS	**CMAQ**	**AURAMS**	**CMAQ**
no. sites	1245	1247	1245	1247
n	774 946	776 154	20 599	20 635
meas. mean	35.64	35.62	60.77	60.72
mod. mean	42.03	51.46	66.66	70.16
MB	6.38	15.85	5.89	9.44
NMB (%)	17.91	44.50	9.68	15.56
ME	16.25	18.82	16.38	14.29
NME (%)	45.59	52.83	26.96	23.54
% within factor of 2	71.3	70.3	94.5	96.2
r^2	0.393	0.438	0.350	0.505

CMAQ's larger O_3 errors were largely due to its inability to correctly predict night-time lows, as shown in Fig. 3, which shows the time-series' of observed as well as AURAMS-, and CMAQ-modelled O_3 concentrations averaged over all O_3 measurement sites.

Performance statistics for daily peak O_3 is also shown in Table 1. Both models over-predicted the daily peaks with AURAMS having a slightly better NMB of 9.7%, whereas CMAQ had a NMB of 15.6%. In contrast, CMAQ had a slightly lower NME and a higher r^2. Both models did well in

predicting the time of the daily peaks, with AURAMS daily peak concentrations within 3-hours of the measured daily peak 65.2% of the time, while CMAQ was slightly better with a value of 68.8%.

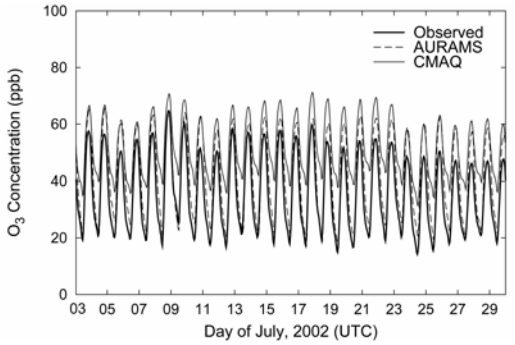

Fig. 3. Site-averaged observed as well as AURAMS-, and CMAQ-modelled O_3 concentrations.

5. COMPARISON OF TOTAL $PM_{2.5}$ PERFORMANCE

Hourly measurement data was taken from the NAPS and AQS networks to evaluate the performance of total $PM_{2.5}$. Statistics are presented in Table 2. Both models under-predicted total $PM_{2.5}$, although AURAMS' under-prediction was much less than CMAQ with a NMB of -15.4% versus -64.5% for CMAQ. However, just as with O_3, the models' errors were more similar, with NMEs of 67.1% and 70.6% for AURAMS and CMAQ, respectively. The similarity in error shows that there was cancellation of positive and negative biases in the AURAMS results, which contributed to the better NMB.

Table 2. AURAMS and CMAQ total $PM_{2.5}$ and daily peak total $PM_{2.5}$ statistics for 3-30 July 2002.

performance statistics	$PM_{2.5}$ ($\mu g\ m^{-3}$)		daily peak $PM_{2.5}$ ($\mu g\ m^{-3}$)	
	AURAMS	CMAQ	AURAMS	CMAQ
no. sites	350	354	350	354
n	211 141	213 707	7444	7538
meas. mean	14.43	14.40	28.26	28.14
mod. mean	12.21	5.11	21.65	9.12
MB	-2.23	-9.29	-6.60	-19.02
NMB (%)	-15.42	-64.52	-23.38	-67.59
ME	9.69	10.16	16.32	19.47
NME (%)	67.12	70.59	57.74	69.18
% within factor of 2	49.8	29.5	59.5	25.8
r^2	0.074	0.151	0.040	0.086

Table 2 also shows the performance statistics for daily peak $PM_{2.5}$. AURAMS performed better with a NMB of -23.4% and NME of 57.7% while CMAQ had a NMB of -67.6% and a NME of 69.2%. CMAQ did slightly better in predicting the time of the daily peaks with 34.2% of modelled $PM_{2.5}$ daily peaks within 3-hours of the measured daily peak, while AURAMS had a value of 28.7%. Station representativeness likely influenced the under-prediction of $PM_{2.5}$ concentrations for both models as most measurement sites were located in urban areas. In addition, the relatively large 42-km grid cells likely caused a "dilution" of $PM_{2.5}$, especially when comparing the modelled concentrations to the high localised concentrations expected around urban centres.

6. COMPARISON OF SPECIATED $PM_{2.5}$ PERFORMANCE

Speciated $PM_{2.5}$ performance was evaluated using 24-hr averaged measurement data from the NAPS network and the U.S. EPA administered Speciation Trends Network (STN).

As shown in Table 3, AURAMS bias was much better than CMAQ for $PM_{2.5}$ sulphate (SO4), ammonium (NH4), and total organic aerosols (TOA), and somewhat worse for nitrate (NO3) and elemental carbon (EC). For NO3, AURAMS over-predicted by approximately 121% while CMAQ under-predicted by approximately 71%. Both models significantly under-predicted TOA concentrations. However, the AURAMS modelled station-mean was over 4 times larger than the CMAQ value, showing better overall TOA performance. This difference was likely due to differences in secondary organic aerosol (SOA) schemes. In addition, the under-prediction in both models was partly due to forest fire emissions not being included in the emissions processing. The inclusion of forest fire emissions would likely improve performance for total PM and TOA.

In terms of error, the AURAMS and CMAQ results were very similar for $PM_{2.5}$ SO4, NH4, and EC, while AURAMS' NME for NO3 was much larger than CMAQ's. For TOA, AURAMS had a better NME of 65.6% versus 91.2% for CMAQ. In terms of correlation, r^2 values for the two models were generally close but CMAQ's were higher.

It is interesting to note that the poor correlation coefficients for both models for total $PM_{2.5}$ (Table 2) may be largely due to their inability in accurately predicting the organic component (Table 3). A large portion of the measured aerosol mass is TOA, while the correlation coefficient for this component is poor for both models.

The differences in AURAMS and CMAQ $PM_{2.5}$ species are likely due to a number of reasons, including differences in the speciation of PM emissions, aerosol chemistry, wet/dry removal mechanisms, and chemical boundary conditions.

Table 3. AURAMS and CMAQ performance statistics for $PM_{2.5}$ sulphate (SO4), nitrate (NO3), ammonium (NH4), elemental carbon (EC), and total organic aerosols (TOA) for 3-30 July 2002.

$PM_{2.5}$ Species	model	no. sites	n	meas. mean ($\mu g\ m^{-3}$)	mod. mean ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	NMB (%)	ME ($\mu g\ m^{-3}$)	NME (%)	% within factor of 2	r^2
SO4	AURAMS	221	1229	5.03	5.31	0.29	5.72	3.03	60.34	57.8	0.367
	CMAQ				2.44	-2.59	-51.51	2.83	56.26	47.2	0.524
NO3	AURAMS	204	1112	0.902	2.00	1.09	121.2	1.58	174.7	30.0	0.397
	CMAQ				0.263	-0.64	-70.87	0.71	79.00	14.8	0.437
NH4	AURAMS	221	1230	1.63	1.64	0.009	0.58	0.885	54.20	60.9	0.428
	CMAQ				0.821	-0.811	-49.68	0.929	56.90	51.2	0.458
EC	AURAMS	205	1180	0.524	0.284	-0.240	-45.83	0.302	57.55	44.7	0.166
	CMAQ				0.338	-0.187	-35.59	0.306	58.42	45.7	0.204
TOA	AURAMS	205	1180	10.56	3.92	-6.64	-62.85	6.93	65.64	33.1	0.0005
	CMAQ				0.928	-9.64	-91.22	9.64	91.25	2.0	0.0066

7. COMPARISON OF PM COMPOSITION

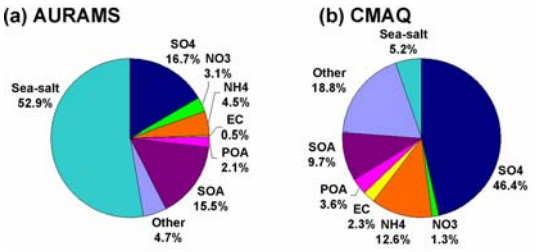

Fig. 4. Average $PM_{2.5}$ composition over all grid cells and last 648 hours of simulation period for (a) AURAMS and (b) CMAQ.

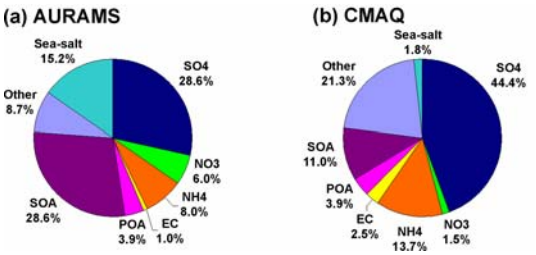

Fig. 5. Average $PM_{2.5}$ composition over land grid cells only and last 648 hours of simulation period for (a) AURAMS and (b) CMAQ.

Fig. 4 shows the average $PM_{2.5}$ composition of AURAMS and CMAQ averaged over all grid cells of their respective domains. The results show very different PM compositions between the models with over 50% of $PM_{2.5}$ mass coming from sea-salt aerosols in AURAMS, whereas only 5.2% of CMAQ's $PM_{2.5}$ mass is from sea-salt aerosols.

As shown in Fig. 5, when the average $PM_{2.5}$ composition is calculated by averaging over land grid cells only, the contribution of sea-salt aerosols to the total mass decreases to 15.2% for AURAMS and 1.8% for CMAQ, showing that sea-salt aerosols contribute a much larger amount to the total PM mass in AURAMS than they do in CMAQ, even if only land grid cells are considered.

8. SUMMARY AND CONCLUSIONS

In general, the two modelling systems showed similar levels of error for O_3, total $PM_{2.5}$, and most $PM_{2.5}$ species. However, in terms of bias, AURAMS performed better for all investigated species, except for $PM_{2.5}$ nitrate. This enhanced bias performance was somewhat due to the cancellation of positive and negative biases as indicated by the similar levels of error.

This study reflects the best effort up to now to closely align many operational aspects of the two modelling systems. However, due to the complexity of the model structures and the numerous interconnected science processes, it is difficult to assess the contributions of individual science processes to the differences in model performance. Improved modularity at the process level would make such scientific process assessment more feasible.

9. NOTE

Results from the brief abstract submitted before and the extended abstract here differ substantially due to incorrect land-use fields generated for the previous AURAMS run. A new AURAMS run was conducted with the correct land-use fields supplied by Environment Canada (EC), and the results are reported in this extended abstract. Investigation is underway to determine the source of the processing error.

10. ACKNOWLEDGEMENTS

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