THE IMPACT OF GEM AND MM5 METEOROLOGY ON CMAQ AIR QUALITY MODELING RESULTS IN EASTERN CANADA AND THE NORTHEASTERN UNITED STATES

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1. INTRODUCTION

As part of a collaborative project between the Institute for Chemical Process and Environmental Technology (ICPET) at the National Research Council of Canada (NRC) and the Canadian Meteorological Centre (CMC) of Environment Canada (EC), a study was conducted to compare and evaluate:

1. meteorological fields generated for a selected nine-day period by two different meteorological models: MM5 and the Global Environmental Multiscale (GEM) model developed by EC (Côté et al., 1998a, b);
2. the emission fields generated using GEM and MM5 meteorology and SMOKE (Houyoux et al., 2003); and
3. the impact of GEM and MM5 meteorology on air quality modeling results from CMAQ.

Except for meteorology, all inputs were identical for the two SMOKE runs. The CMAQ model runs also had identical inputs, except for meteorology and those emissions dependent on meteorology. The two sets of meteorological, emissions, and air quality model results were then analyzed to show the differences resulting from the use of the different meteorological inputs.

2. MODELING SYSTEM

2.1. Meteorological Models and Setup

GEM v3.1.1 with physics v4.0 was run by CMC and used 28 hybrid coordinate levels, a model top of 10 hPa and a 190×190 domain with 24-km grid spacing.

MM5 v3.3, run by RWDI Inc. (2002) and transferred to NRC by the Ontario Ministry of Environment (OME), was used with 27 vertical sigma layers, a model top of 100 hPa and two nested domains consisting of an 85×64 inner domain with 36-km grid spacing.

Both GEM and MM5 results were processed and converted to SMOKE- and CMAQ-ready meteorological input files through GEM-MCIP, a meteorology processor developed at NRC as an extension of the U.S. EPA's Meteorology-Chemistry Interface Program (MCIP) with the added capability to read and process GEM meteorological fields as well as the standard MM5 meteorological files.

2.2. Emissions

SMOKE v2.0 was used in this study to create CMAQ-ready Canadian and U.S. emission files. Canadian point, area and non-road mobile sources emissions were generated using the 1995 raw emissions inventory developed by EC, while on-road mobile emission files were generated using 1999 provincial vehicle miles traveled (VMT) data provided by SENES/AIR (2002), MOBILE6.2C (SENES/AIR, 2004), and GEM and MM5 meteorological files for the simulation period.

U.S. emission files for point, area and non-road mobile sources were generated using version 3 of the 1999 National Emissions Inventory (NEI) released by the U.S. EPA, while on-road mobile emission files were generated using 1999 VMT data from the 1999 NEI, MOBILE 6.2, and GEM and MM5 meteorological files.

Biogenic emission files for both Canada and the U.S. were generated using BEIS v3.09, a BELD3 land-use dataset for the domain, and GEM and MM5 meteorological files.

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2.3. Air Quality

CMAQ v4.3 was used in this study with a modified version of the RADM2 chemical mechanism (Stockwell et al., 1990), named "radm2_ci1_ae2_aq", for gas phase chemistry, along with the “qssa” chemistry solver and the “aero2” aerosol module.

The NRC PMx software package (Jiang and Yin, 2001) was used as a CMAQ post-processor to calculate size distribution parameters and PM concentrations within required particle size ranges from the CMAQ output tri-modal PM concentrations. Calculations were done on the basis of classical aerodynamic diameter (Jiang et al., 2004) to facilitate comparison with field measurement data.

2.4. Modeling Domain and Simulation Period

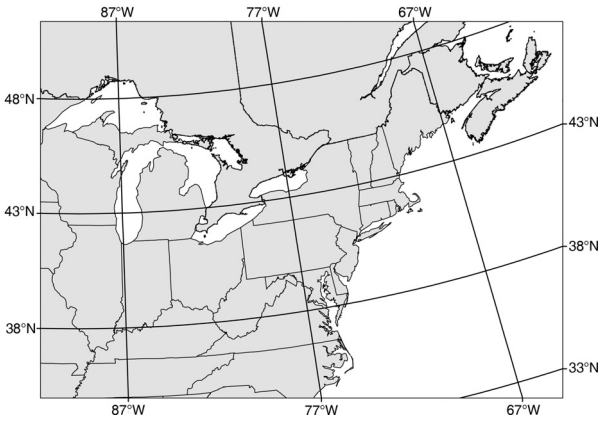

Fig. 1. Horizontal modeling domain.

The horizontal modeling domain shown in Fig. 1 is on a Lambert Conformal Conic projection, covers 5 Canadian provinces and 27 U.S. states, and consists of a 68×49 grid with 36-km resolution. Vertically, 15 terrain-following sigma layers were used. The modeled time period is from 0000 UTC 11 July 1999 to 2300 UTC 19 July 1999 with a widespread ozone and PM episode occurring through eastern Canada and the northeastern U.S. midway through this period.

3. COMPARISON OF GEM AND MM5 METEOROLOGY

Table 1 presents comparison statistics between selected GEM and MM5 meteorological fields investigated in this study.

The modeled pressures and temperatures for GEM and MM5 match each other very well with normalized mean differences (NMDs) of less than 1% for pressure and less than 6% for temperature. Wind speed comparison shows that GEM wind speeds are on average 0.6 m s^{-1} greater than MM5 with a NMD of 15.0%, while GEM relative humidity (RH) values are on average 11% higher than MM5 with a NMD for RH of 16.6%. In subsequent sections the differences in RH will be shown to play a significant role in the differences in CMAQ predicted aerosol concentrations.

4. IMPACT OF METEOROLOGY ON EMISSIONS

SMOKE v2.0 was run twice for all emission sources, including area, point, biogenic, on-road mobile, and non-road mobile sources, using GEM meteorology for one run and MM5 for the other. In SMOKE, biogenic, point, and on-road mobile sources require meteorology as an input for generating emissions while area and non-road mobile sources do not require meteorological inputs and thus are identical in the two SMOKE runs. Emissions from biogenic and on-road mobile sources occur only at ground level and need not be evaluated at upper vertical layers. However, point source emissions are distributed vertically and must be analyzed accordingly.

Table 1. Comparison statistics of all GEM and MM5 surface-level pressure, temperature, wind speed and relative humidity pairs for the entire simulation period.

model results	pressure (hPa)		temperature (°C)		wind speed (m s^{-1})		RH (%)	
	GEM	MM5	GEM	MM5	GEM	MM5	GEM	MM5
n	719 712	719 712	719 712	719 712	745 200	745 200	719 712	719 712
mean	996.6	995.6	21.4	22.7	4.6	4.0	78.7	67.5
standard deviation	21.4	21.6	4.5	4.8	2.6	2.1	13.4	18.2
comparison statistics								
MD [a]	1.0 hPa		-1.3 °C		0.6 m s^{-1}		11.2 %	
NMD (%) [b]	0.1 %		-5.6 %		15.0 %		16.6 %	
NAD (%) [c]	0.2 %		10.1 %		35.9 %		21.5 %	

[a] mean difference (MD) = $^1/_n \Sigma$(GEM-MM5); [b] normalized mean difference (NMD) = [Σ(GEM-MM5) / Σ(MM5)] × 100%;
[c] normalized absolute difference (NAD) = [Σ|GEM-MM5| / Σ(MM5)] × 100%

Table 2. Summary of GEM and MM5 on-road mobile, biogenic, and total emissions (metric kilotons) from all sources summed over the entire modeled domain and simulation period as well as the relative difference (RD) in emissions.

pollutant	on-road mobile emissions			biogenic emissions			total emissions		
	GEM	MM5	RD[a] (%)	GEM	MM5	RD (%)	GEM	MM5	RD (%)
CO	837.4	836.7	0.1	-	-	-	1269.0	1268.4	0.1
VOC	85.5	88.4	-3.3	880.5	1056.1	-16.6	1090.9	1269.4	-14.1
NOx	121.6	122.0	-0.3	8.1	9.2	-11.8	248.6	250.1	-0.6
TPM	3.0	3.0	0	-	-	-	74.4	74.4	0
NH3	3.3	3.3	0	-	-	-	45.9	45.9	0
SOx	4.1	4.1	0	-	-	-	178.4	178.4	0
TOTAL	1062.9	1065.4	-0.2	888.6	1065.3	-16.6	2948.2	3127.4	-5.7

[a] Relative Difference (RD) = (GEM – MM5) / MM5 × 100%.

Table 2 compares carbon monoxide (CO), volatile organic compounds (VOC), nitrogen oxide (NO_x), total particulate matter (TPM), ammonia (NH_3), and sulfur oxide (SO_x) emissions from on-road mobile sources and biogenic sources, as well as total emissions from all sources summed over all horizontal grid cells, all vertical layers, and all 216 hours of the simulation period.

4.1. On-road Mobile Emissions

On-road mobile emissions are generated using an adapted version of the MOBILE6.2/6.2C models, which calculate emission factors using surface temperature as the only meteorological input. Therefore, the differences in on-road mobile emissions based on GEM and MM5 (called 'GEM emissions' and 'MM5 emissions' later for brevity) are a direct result of the temperature differences between the two models.

Total MM5 on-road mobile emissions of VOC and NO_x are greater than GEM emissions by 3.3% and 0.3%, respectively. GEM on-road mobile emissions of CO are 0.1% greater than MM5. Overall, GEM on-road mobile emissions are 0.2% less than MM5 showing that the minor temperature difference of 1.3°C between the models has a correspondingly minor effect on the on-road mobile source emissions.

4.2. Biogenic Emissions

Biogenic emissions were generated using BEIS v3.09, which calculates correction factors for biogenic emissions of monoterpenes (MONO), isoprene (ISOP), other VOCs (OVOC), and nitric oxide (NO). Surface temperature is the only required meteorological input to the BEIS model necessary to generate the MONO, OVOC and NO correction factors, while ISOP requires surface temperature and photosynthetically active radiation (PAR) (Pierce et al., 1998).

The relative difference (RD) of 11.8% between GEM and MM5 biogenic NO emissions is the direct result of differences in GEM and MM5 surface temperatures. This shows that the small mean difference of 1.3°C between GEM and MM5 surface temperature has a much larger effect on biogenic NO_x emissions than on on-road mobile source NO_x emissions.

The influence of the temperature difference between the models is even larger for biogenic VOC emissions. The use of MM5 meteorology increases biogenic VOC emissions by approximately 175 000 metric tons over the GEM meteorology, resulting in a relative difference of 16.6%. This variation is mainly attributable to the difference in temperature, although solar radiation differences also have some impact.

4.3. Point Source Emissions

The total amount of pollutant emissions from point sources is dependent only on the amount in the raw inventory and does not change with meteorology. However, the distribution of point source emissions is affected by wind speed and direction and other factors affecting plume rise and pollutant dispersion.

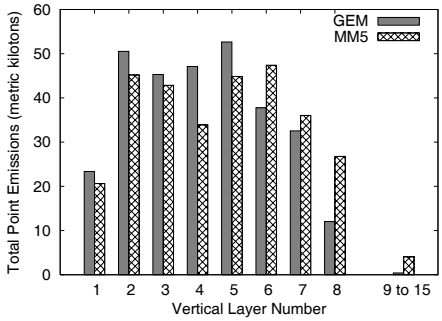

Fig. 2. Vertical distribution of total point source emissions by CMAQ layer number.

As seen in Fig. 2, within the first five vertical layers GEM total point source emissions are

greater than MM5 emissions, with relative differences ranging from 5.7% greater in the third vertical layer to 38.9% in the fourth vertical layer. Conversely, in layers 6 through 15, GEM emissions are less than MM5, with relative differences ranging from 9.7% less in layer 7 to 93.8% less in layer 13.

5. IMPACT OF METEOROLOGY ON CMAQ RESULTS

5.1. O_3, PM_{10}, and $PM_{2.5}$

Table 3 presents comparison statistics for modeled O_3 and shows that the average GEM and MM5 O_3 concentrations are very similar. The mean GEM O_3 concentration is about 0.8 ppb less than the mean MM5 concentration, corresponding to a NMD of only -1.7%. The combined effects of increased temperature in the MM5 model resulting in increased isoprene and NO_x emissions are likely the main reasons for the higher average MM5 O_3 concentrations.

Table 3 also presents the comparison statistics for GEM and MM5 ground-level PM_{10} concentrations over all grid cells and time steps. On average GEM PM_{10} concentrations are higher than MM5 concentrations with a mean difference of 4.0 μg m^{-3}, corresponding to a NMD of 41.2%. In comparison, the NMD between GEM and MM5 $PM_{2.5}$ concentration is much smaller at 6.0%.

The increase in RD as particle diameter cut-off increases is largely the result of the influence of RH. Within the CMAQ model, higher RH tends to result in increased total particle mass, increased particle diameters, and an increased contribution of particle-bound water (AH2O) to the total particle mass (Jiang et al., 2005). And as shown in Table 1, GEM predictions of RH were higher on average than MM5 predictions.

Fig. 3a shows total (i-mode + j-mode + c-mode) modeled particle mass distribution curves at ground-level, based on classical aerodynamic diameter (D_{ca}), averaged over the entire domain and simulation period for both GEM and MM5. The overall shapes of the curves are very similar; however they differ in two significant ways. First, the peak of the GEM distribution approaches 5.0 μg m^{-3} while for MM5 the peak is smaller at around 3.0 μg m^{-3}. Secondly, the position of the curves along the x-axis is slightly different. The MM5 distribution curve peaks to the left of the 2.5 μm cut-off line, while the GEM distribution curve peaks to the right of the 2.5 μm cut-off line and shows that the bulk of the total GEM PM mass is contained in particles larger than 2.5 μm in diameter.

The differences in the PM mass distribution curves affect the average GEM and MM5 $PM_{2.5}$ and PM_{10} concentrations as calculated by the NRC PMx software. The main reason for these differences is the higher average RH in the GEM model and its influence on total PM mass and the particle size of all PM species.

This becomes more evident when comparing 'wet' particle mass distributions (Fig. 3a) to the 'dry' distributions (Fig. 3b). The 'dry' mass distribution curves are calculated in the same manner as the 'wet' distributions but exclude AH2O from the calculation of total PM mass. The GEM and MM5 'dry' mass distribution curves are more similar than the 'wet' PM distributions, although the GEM distribution still has a slightly higher peak and is shifted slightly towards the larger diameters. This suggests that the higher RH in the GEM model not only affects the size and concentration of the AH2O aerosol species, but the other aerosol species as well.

Table 3. Comparison statistics of all GEM and MM5 surface-level ozone, PM_{10}, and $PM_{2.5}$ pairs for the entire simulation period (n = 719 712).

model results	O_3 (ppb)		PM_{10} (μg m^{-3})		$PM_{2.5}$ (μg m^{-3})	
	GEM	MM5	GEM	MM5	GEM	MM5
mean	44.4	45.2	13.6	9.6	6.9	6.5
standard deviation	17.7	15.9	17.6	11.5	8.1	7.4
comparison statistics						
MD	-0.8		4.0		0.4	
NMD (%)	-1.7 %		41.2 %		6.0 %	
NAD (%)	15.9 %		68.7 %		44.4 %	

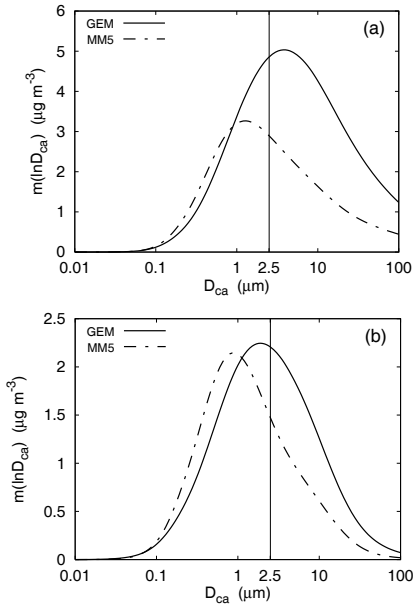

Fig. 3. GEM and MM5 modeled total particle mass distribution curves averaged over entire domain and simulation period: (a) 'wet' total PM mass (i.e. includes AH2O); (b) 'dry' total PM mass (i.e. excludes AH2O).

5.1.2. RH Sensitivity Test

Although differences in several meteorological fields have been investigated in this study, there are dozens of meteorological parameters passed from the models that are likely to be different and impact air quality. In order to confirm the above discussion of the role of RH on particle sizes and concentrations, a sensitivity test was performed using the GEM-based meteorology, emissions, etc. as the base case for the same modeled domain and the first 2-days of the simulation period. Water vapor mixing ratio was reduced by 25% (corresponding to ≈ 25% reduction in RH) for the sensitivity case. Comparison of the results showed that the total 'dry' and 'wet' mass distributions were shifted towards smaller diameters for the sensitivity case, which had lower RH, reinforcing the previous discussion concerning the effect of RH on particle sizes.

5.2. Speciated PM

Table 5 shows the PM_{i+j}, $PM_{2.5}$ and PM_{10} concentrations for all fine CMAQ PM species, including sulfate (ASO4), nitrate (ANO3), ammonium (ANH4), primary anthropogenic organic matter (AORGPA), secondary anthropogenic organic matter (AORGA), secondary biogenic organic matter (AORGB), elemental carbon (AEC), particle-bound water (AH2O), and other fine particulates (A25).

Overall, the differences in $PM_{2.5}$ species are qualitatively similar. Except for AH2O and ANO3, all species have a negative RD, meaning that MM5 concentrations are greater on average than GEM concentrations. The large difference in AH2O concentrations is directly related to the differences in RH between the two models (Jiang et al., 2005).

It is interesting to note that the magnitudes of the relative difference between the GEM and MM5 average ASO4, ANO3, ANH4, and AH2O PM_{i+j} concentrations are much higher than the other PM species. The larger relative difference in AH2O concentration is due to the difference in RH, while the larger differences in ASO4, ANO3, and ANH4 concentrations could be due to a variety of factors including aqueous chemistry and/or thermodynamic equilibrium.

5.3. CMAQ Configuration Sensitivity Test

Upon completion of this study, equivalent analysis was completed using CMAQ version 4.4 with the 'radm2_ci4_ae3_aq' chemical mechanism and the "aero3" module for aerosol modeling. Although the statistics did change and PM concentrations were lower, qualitatively, the results and conclusions are the same.

Table 5. Comparison of GEM and MM5 surface-level PM_{i+j}, $PM_{2.5}$, and PM_{10} species concentrations averaged over the entire modeled domain and simulation period.

	PM_{i+j} (μg m^{-3})			$PM_{2.5}$ (μg m^{-3})			PM_{10} (μg m^{-3})		
	GEM	MM5	RD (%)	GEM	MM5	RD (%)	GEM	MM5	RD (%)
ASO4	3.92	2.86	36.8	1.75	1.96	-10.7	3.07	2.62	17.3
ANO3	0.331	0.180	83.6	0.136	0.119	14.2	0.244	0.162	50.7
ANH4	1.08	0.849	27.8	0.508	0.615	-17.4	0.871	0.797	9.3
AORGPA	0.182	0.177	2.8	0.091	0.133	-31.7	0.150	0.168	-10.6
AORGA	0.250	0.234	6.9	0.130	0.177	-26.8	0.205	0.221	-6.9
AORGB	0.537	0.665	-19.2	0.312	0.523	-40.2	0.459	0.630	-27.1
AEC	0.153	0.146	4.1	0.076	0.110	-31.3	0.126	0.139	-9.8
A25	0.784	0.737	6.4	0.383	0.552	-30.5	0.643	0.701	-8.2
AH2O	13.1	5.74	128.0	3.44	2.25	52.7	7.37	3.76	95.9

6. CONCLUSIONS

Different results from meteorological models are to be expected. However, the impact of meteorological differences on air quality modeling is difficult to quantify fully due to the complex chemistry and physics that take place in the modeled atmosphere. Nonetheless, the differences in air quality predictions found in this study as a result of the use of meteorological datasets produced by two different models suggests that these impacts can be pervasive and constitute a significant source of variance.

Overall, this study has shown that the use of GEM meteorology in SMOKE emissions modeling/processing and CMAQ air quality modeling, for the eastern Canada and northeastern U.S. domain and July 1999 simulation period produces results comparable to MM5 meteorology.

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