TWO YEARS OF OPERATIONAL AQ FORECASTING WITH GEM-MACH15: A LOOK BACK AND A LOOK AHEAD

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1. INTRODUCTION

GEM-MACH15 (Global Environmental Multiscale model-Modelling Air quality and CHemistry at 15 km) has been Environment Canada's (EC) operational regional air quality (AQ) forecast model since it replaced the CHRONOS AQ model in November 2009 after a three-month test period. GEM-MACH15 (abbreviated G-M15) is a limited-area configuration of GEM-MACH, an on-line chemical transport model that is embedded within GEM, EC's multi-scale operational weather forecast model. The operational version of GM15 is run twice daily at EC's Canadian Meteorological Centre to produce 48-hour AQ forecasts on a North American grid (Anselmo et al., 2010).

G-M15 forecasts provide important guidance to the Canadian AQ forecast program, whose key product is the national Air Quality Health Index (AQHI) for urban areas. The AQHI is a health-based, additive, no-threshold, hourly AQ index with a 0 to10+ range that is based on a weighted sum of local O_3, $PM_{2.5}$, and NO_2 concentrations. It was developed from a time-series analysis of air pollutant concentrations and mortality in Canadian cities (Stieb et al., 2008). Although G-M15 predicts hourly concentration fields of many gas-phase and size-specific particle-phase species, the three most important fields are O_3, $PM_{2.5}$, and NO_2, needed for the AQHI.

The G-M15 forecast system has now been running operationally for more than two years but has undergone several modifications during that period (Sec. 2). This paper presents selected statistical analyses of model performance during this period and notes some impacts of model changes on model performance (Sections 3-5). G-M15 post-processing and future plans are then discussed in Sections 6 and 7.

2. FORECAST SYSTEM DESCRIPTION

A number of AQ process representations from EC's AURAMS (A Unified Regional Air-quality Modelling System) off-line chemical transport model (e.g., Gong et al., 2006) have been implemented in GEM-MACH, including those for gas-phase, aqueous-phase, and heterogeneous chemistry and for a number of PM processes (nucleation, condensation, coagulation, inorganic gas-particle partitioning, sedimentation and dry deposition, in-cloud and below-cloud scavenging, and secondary organic aerosol (SOA) formation) (Talbot et al., 2008; Anselmo et al., 2010).

GEM-MACH employs a simple 2-bin sectional representation of the PM size distribution (Bin 1 is 0-2.5 μm aerodynamic diameter and Bin 2 is 2.5-10 μm), but PM chemical composition is treated in more detail. Nine chemical components are considered: SO_4, NO_3, NH_4, elemental carbon (EC), primary organic aerosol (POA), SOA, crustal material, sea salt, and particle-bound water.

The SMOKE emissions processing system v2.6 was used to produce anthropogenic input emissions files on the G-M15 grid from the 2006 Canadian, 2005 U.S., and 1999 Mexican national emissions inventories. Biogenic emissions are estimated on-line using the BEIS v3.09 algorithms. Note that neither wildfire or Aeolian dust emissions are considered in the current version of G-M15, nor is the meteorological modulation of fugitive dust emissions.

G-M15 is a limited-area configuration of GEM-MACH. Horizontally, a 348 x 465 rotated latitude-longitude grid spanning a North American continental domain with 15-km grid spacing is used (see Fig. 1), and 58 vertical levels extend from the surface to 0.1 hPa on a hybrid vertical coordinate. As a coupled meteorology-chemistry model, G-M15 predicts the time evolution of both

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meteorological and chemical fields, but time-dependent meteorological lateral boundary conditions (LBCs) are provided to G-M15 by GEM-LAM15, EC's limited-area version of GEM with 15-km horizontal grid spacing that is used for operational two-day regional weather forecasts (see Fig. 1). Average concentration vertical profiles for different species are used to provide chemical LBCs: seasonal profiles for O_3 and CO, annual profiles for other model species. Chemical fields are initialized for each 48-h simulation by cycling the 12-h forecast of the previous model run.

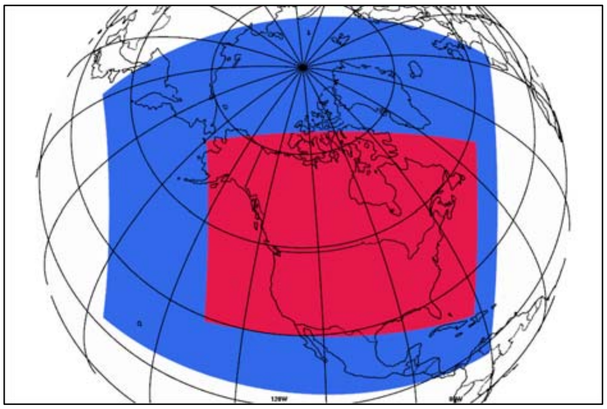

Fig. 1. Positions of GEM-LAM15 grid (blue) and embedded GEM-MACH15 grid (red).

The operational G-M15 forecasting system has undergone two upgrades since June 2009 when it first went into service in "parallel" (evaluation) mode. In March 2010 a revised set of emissions files were introduced to solve a problem with $PM_{2.5}$ overpredictions in some Canadian provinces (see Moran et al., 2010), and in Oct. 2010 the meteorological model supplying meteorological LBCs to G-M15 was changed from a global variable-grid configuration of GEM15 to the limited-area GEM-LAM15. The latter change had little impact, but as discussed in Sec. 5, the change in primary $PM_{2.5}$ emissions was evident in model performance evaluation scores.

3. DATA SOURCES

An archived set of near-real-time (NRT) hourly measurements of O_3, $PM_{2.5}$, and NO_2 surface concentrations obtained from Canadian National Air Pollution Surveillance (NAPS) network stations (via EC's Automatic Data Extraction circuit) and O_3 and $PM_{2.5}$ surface concentrations obtained from U.S. stations (via AIRNow: see http://airnow.gov) from 2009 to 2011 have been used to evaluate G-M15 performance over this period. The NRT data from Canadian stations have not undergone extensive quality control checks by individual networks, but they have been filtered for this study for outliers. For example, it appears that some stations report calibration data as actual measurements. To screen out such values, cutoff thresholds of 220 ppbv, 220 µg m^{-3}, and 100 ppbv were applied to O_3, $PM_{2.5}$, and NO_2 hourly observations, respectively. The filter removed less than 0.1% of all available hourly data over the two-year period.

As shown in Table 1, O_3, $PM_{2.5}$, and NO_2 measurements at up to 1,312, 770, and 133 stations, respectively, are available for North America during the 2009-11 period. While Canadian air-quality stations and U.S. $PM_{2.5}$ stations operate year-round, Table 1 shows that many U.S. O_3 stations only operated during the "ozone season" from May to September.

The locations of the stations measuring O_3, $PM_{2.5}$, and NO_2 can be seen in Figs. 2a, 2b, and 2c, respectively. It is evident from these plots that the spatial distribution of monitoring stations is not uniform, with less dense coverage over central and northern Canada and the central U.S. (e.g., Alberta vs. Manitoba, Ohio vs. Nebraska). The number of monitors available for each Canadian province for these three species is also listed in the first column of Tables 2 to 4. Note that the evaluation statistics for some provinces are based on as few as three monitors, and in the case of the Northwest Territories (NT), one monitor.

Table 1. Minimum number of available Canadian and U.S. stations in 2009-2011 measuring O_3, $PM_{2.5}$, and NO_2 in the cold-season (Oct.–Mar.) and warm-season (Apr.–Sept.) periods.

Country/Species	O_3	$PM_{2.5}$	NO_2
Canada summer	184	170	134
Canada winter	182	171	133
U.S. summer	1,128	597	N/A
U.S. winter	626	599	N/A

4. EVALUATION METHODOLOGY

A new model performance evaluation package called VAQUM ("Verification of Air QUality Models") has been used to store measured and modelled station values and to calculate various evaluation metrics (Gilbert et al., 2010). This package is based on the PostgresSQL (v9.0) relational database system with the PostGIS spatial processing extension.

The evaluation period that was considered was the two-year period from 1 Aug. 2009 to 31 July 2011. In order to compare model performance between different years, statistics were calculated for two 12-month periods, namely the period 1 Aug. 2009 to 31 July 2010, hereafter referred to as "Year 1", and 1 Aug. 2010 to 31 July 2011, hereafter referred to as "Year 2".

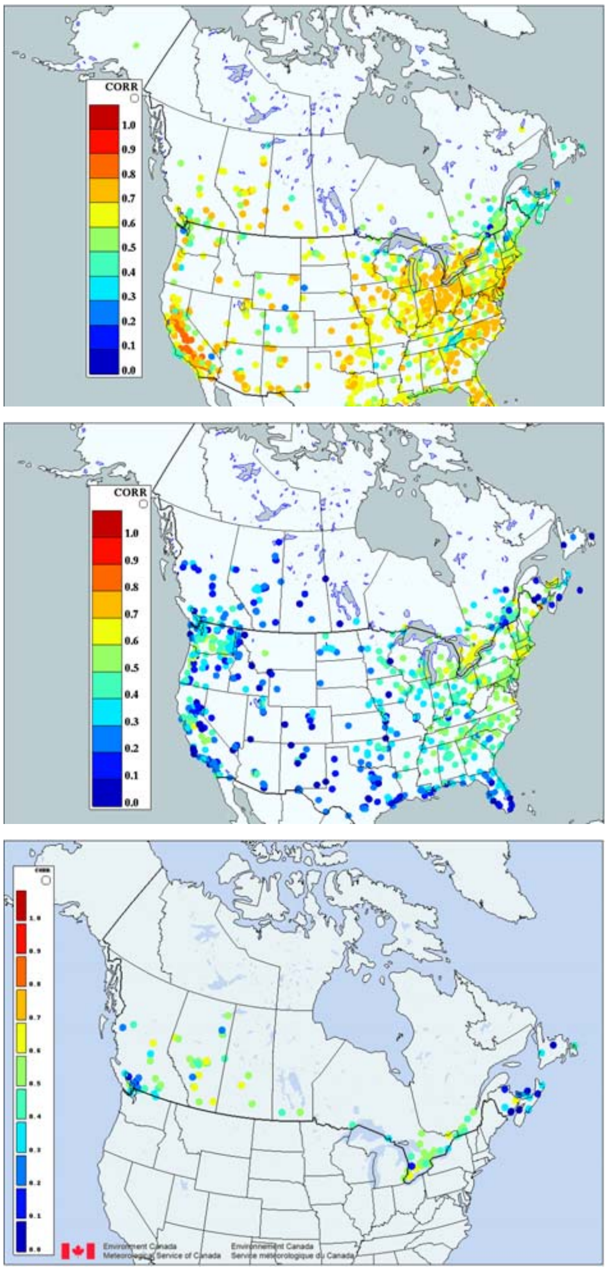

Fig. 2. Year 1 annual correlation (R) values at Canadian and U.S. measurement stations for hourly O_3 (top panel), $PM_{2.5}$ (middle panel), and NO_2 (bottom panel) concentrations.

Table 2. Selected annual statistics for daily maximum hourly O_3 by province and country for Years 1 and 2. Number of monitors is listed after each Canadian province's abbreviation (197 monitors for Canada, 1,204 for U.S. in 2010)

Metric	**ObsAvg (ppbv)**		**MB (ppbv)**		**RMSE (ppbv)**		**R**	
Region	**Y1**	**Y2**	**Y1**	**Y2**	**Y1**	**Y2**	**Y1**	**Y2**
BC 35	32	33	0.1	-1.7	11	10	0.54	0.52
AB 30	36	37	-3.2	-6.3	11	12	0.63	0.60
SK 5	32	38	-0.9	-5.9	13	10	0.49	0.64
MB 3	33	37	-1.9	-5.0	10	10	0.60	0.57
ON 42	40	40	-0.5	-0.1	13	12	0.68	0.72
QC 50	35	36	-0.5	-1.0	12	11	0.53	0.56
NB 14	34	34	1.0	1.1	11	11	0.33	0.39
PE 3	36	35	-2.0	-1.4	9	10	0.39	0.34
NS 10	34	36	2.1	-0.1	14	12	0.29	0.35
NL 4	35	35	-4.0	-4.1	10	10	0.25	0.34
NT 1	36	35	-7.0	-6.1	9	9	0.63	0.56
CAN	35	36	-0.7	-1.8	12	11	0.58	0.58
USA	46	47	4.3	3.7	19	20	0.59	0.60

Table 3. Same as Table 2 but for $PM_{2.5}$ (190 monitors for Canada, 661 for U.S. in 2010)

Metric	**ObsAvg ($\mu g\ m^{-3}$)**		**MB ($\mu g\ m^{-3}$)**		**RMSE ($\mu g\ m^{-3}$)**		**R**	
Reg\Yr	**Y1**	**Y2**	**Y1**	**Y2**	**Y1**	**Y2**	**Y1**	**Y2**
BC 48	12	13	2.6	0.6	21	22	0.03	0.00
AB 30	16	18	9.0	-0.8	40	29	0.24	0.15
SK 4	14	15	11.4	-0.3	46	22	0.01	0.03
MB 4	15	13	2.6	4.0	21	20	0.15	0.10
ON 37	12	12	15.3	13.9	26	23	0.47	0.56
QC 45	17	17	15.1	10.0	40	28	0.27	0.45
NB 8	17	15	-7.1	-5.2	28	16	0.10	0.30
PE 3	10	10	-2.1	-1.7	8	9	0.57	0.47
NS 8	15	17	-4.4	-6.7	28	29	0.02	0.05
NL 3	18	15	-7.1	-4.6	38	24	0.00	0.12
CAN	14	15	8.7	4.9	32	25	0.21	0.23
USA	18	18	8.5	7.3	26	25	0.30	0.30

Table 4. Same as Table 2 but for NO_2 (150 monitors in Canada in 2010).

Metric	**ObsAv ($\mu g\ m^{-3}$)**		**MB ($\mu g\ m^{-3}$)**		**RMSE ($\mu g\ m^{-3}$)**		**R**	
Reg\Yr	**Y1**	**Y2**	**Y1**	**Y2**	**Y1**	**Y2**	**Y1**	**Y2**
BC 36	18	17	-0.2	-1.9	13	12	0.57	0.52
AB 35	18	17	9.9	8.9	18	17	0.57	0.56
SK 4	21	20	-0.5	2.0	11	12	0.56	0.50
MB 3	17	18	3.5	4.0	11	12	0.53	0.55
ON 33	20	19	4.9	3.3	14	13	0.60	0.62
QC 21	19	21	9.3	8.9	17	17	0.53	0.59
NB 6	11	11	0.9	0.0	12	11	0.27	0.35
PE 3	6	6	-2.5	-0.6	6	6	0.59	0.56
NS 6	11	11	-1.3	-1.8	12	11	0.47	0.43
NL 3	9	9	-4.3	-6.2	9	10	0.46	0.48
CAN	18	17	4.5	3.6	15	14	0.57	0.58

5. EVALUATION RESULTS

There are numerous evaluation metrics that can be calculated. This section presents results for some selected metrics that characterize overall model performance by species, by time period, and by region. These evaluation results for the first two years of G-M15 operation will provide a basis for comparison with model performance for future model versions. Some metrics consider all hourly values and some focus on maximum hourly values, since model performance for both average and extreme conditions is of interest.

5.1 Annual Statistics by Region

Tables 2 to 4 summarize three standard statistical measures, mean bias (MB), root mean square error (RMSE), and correlation coefficient (R), for individual Canadian provinces and for Canada and the U.S. for Years 1 and 2 for daily maximum hourly O_3, $PM_{2.5}$, and NO_2 concentrations, respectively.

A comparison of the statistics for the three species suggests that G-M15 performs best for daily maximum O_3 and worst for daily maximum $PM_{2.5}$. For example, Year 1 and Year 2 R values for Canada are O_3: 0.58 and 0.58, $PM_{2.5}$: 0.21 and 0.23, and NO_2: 0.57 and 0.58. The corresponding values of normalized mean bias (NMB = MB/ObsAvg) are O_3: -2% and -5%, $PM_{2.5}$: 60% and 34%, and NO_2: 26% and 21%, and the corresponding values of the coefficient of variation of the RMSE (defined as RMSE/ObsAvg) are O_3: 0.33 and 0.31, $PM_{2.5}$: 2.21 and 1.69, and NO_2: 0.84 and 0.82, respectively.

Examination of the three tables also reveals considerable spatial variation in model performance. For example, the range in annual R values between Canadian provinces goes from 0.25 (NT) to 0.72 (ON) for daily maximum O_3, from 0.00 (BC, NL) to 0.57 (PE) for daily maximum $PM_{2.5}$, and from 0.27 (NB) to 0.62 (ON) for daily maximum NO_2. In fact annual R values are very low for daily maximum $PM_{2.5}$ for a number of provinces, illustrating the challenge presented by this pollutant.

Figure 2 presents another view of the spatial variation of G-M15 performance for annual R values of O_3, $PM_{2.5}$, and NO_2, but in this case by individual station and for all hours of the day. Interestingly, although it is evident from this figure that model performance can and does vary between neighbouring stations, the larger variations in performance tend to be between regions.

Examination of Tables 2 to 4 also suggests that overall model performance is very similar for Year 1 vs. Year 2. The one exception is for $PM_{2.5}$, where Year 2 scores are markedly better for some Canadian provinces. For example, MB is reduced from 9.0 to -0.8 μg m^{-3} for Alberta, from 11.4 to -0.3 μg m^{-3} for Saskatchewan, from 15.1 to 10.0 μg m^{-3} for Quebec, and from 8.7 to 4.9 μg m^{-3} for Canada. The reason for this improvement was the introduction of an improved set of Canadian primary $PM_{2.5}$ emissions in March 2010, as described by Moran et al. (2010).

5.2 National Annual Time Series

Figure 3 shows four sets of time series of predicted and observed mean daily maximum 1-hour ozone concentrations, two for Canadian stations for Year 1 and Year 2 and two for U.S. stations for the same two periods. It is evident that G-M15 has a tendency to overpredict O_3 during the warm season (April–Sept.) and to underpredict it during the cold season (Oct.–Mar.). The warm-season positive bias is also larger over the U.S. than Canada. Similar behaviour can be seen for each of the two 1-year periods.

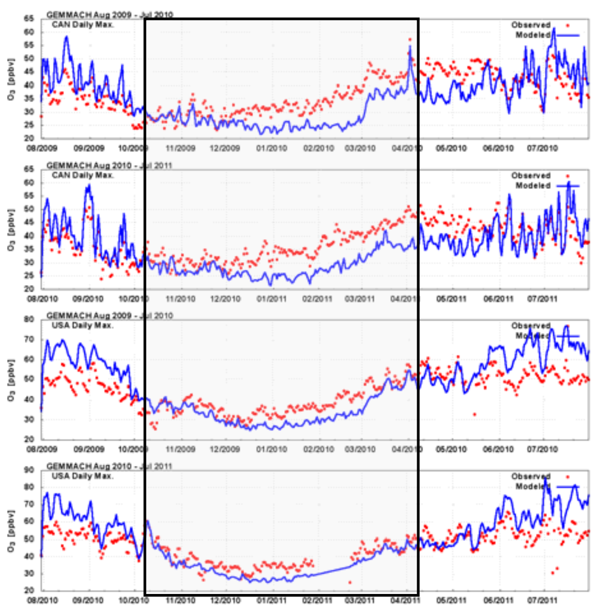

Fig. 3. Annual time series of predicted and measured national-average daily maximum one-hour ozone concentrations (ppbv) at Canadian stations for (a) 2009-10 and (b) 2010-11 periods and at U.S. stations for (c) 2009-10 and (d) 2010-11 periods. The light-gray stippled area indicates the cold-season period from 1 October to 31 March.

Figure 4 shows comparable sets of time series for predicted and observed mean daily maximum

1-hour $PM_{2.5}$ concentrations. Interestingly, this figure suggests that G-M15 tends to overpredict $PM_{2.5}$ at all times of year. The warm-season positive bias is again larger for the U.S. than Canada, and again, the time series for Year 1 and Year 2 are qualitatively similar. The larger cold-season overpredictions over Canada for Year 1 vs. Year 2 before and after the introduction of the new emissions files in March 2010 are also visible.

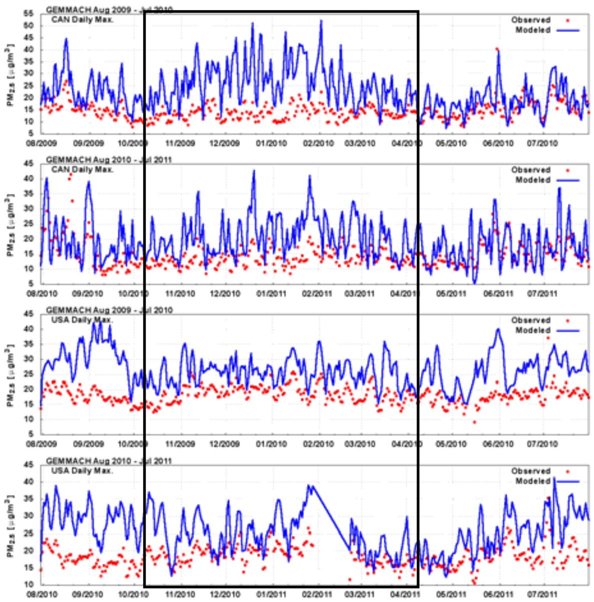

Fig. 4. Same as Fig. 3 but for national-average daily maximum one-hour $PM_{2.5}$ concentrations (μg m^{-3}).

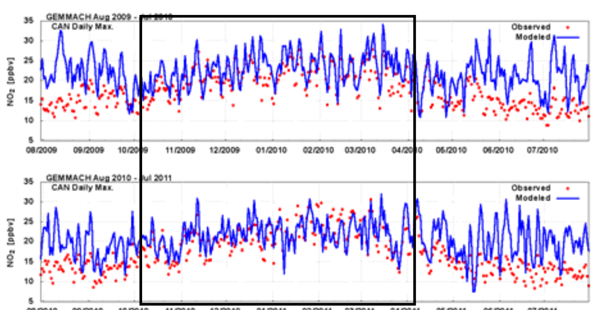

Fig. 5. Same as Fig. 3 but for national-average daily maximum one-hour NO_2 concentrations (ppbv) for Canada only.

Figure 5 shows comparable sets of time series for predicted and observed mean daily maximum 1-hour NO_2 concentrations at Canadian stations only. For NO_2 the G-M15 predictions are similar to measured Canada-mean values in the cold season but too high in the warm season. This same behaviour is seen for both forecast years.

5.3 Seasonal and Regional Variation of Model Errors

It is also of interest to examine how model statistics such as MB, NMB, RMSE, and R vary by time of the year and by region. Figure 6 shows a simple geometric division of the model grid (over land) into four large regions: western and eastern Canada and western and eastern U.S. Mean monthly model errors have been calculated for the measurement stations in each of these four regions for the full two-year period from August 2009 to July 2011.

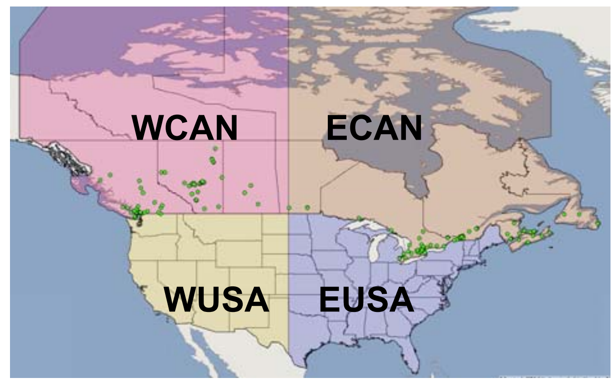

Fig. 6. Four quadrants used for regional analyses, where "WCAN" denotes "Western Canada", "ECAN" denotes "Eastern Canada", "EUSA" denotes "Eastern U.S.A.", and "WUSA" denotes "Western U.S.A.".

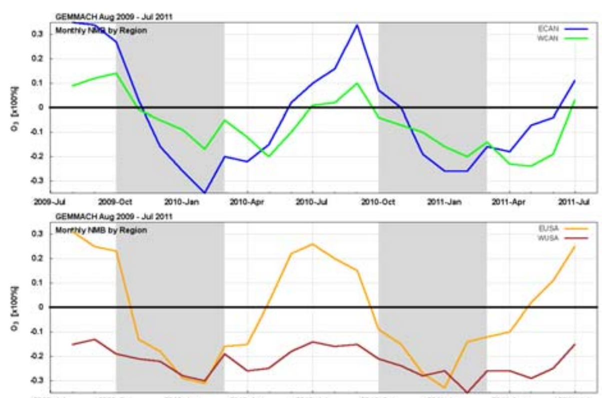

Fig. 7. Monthly variation of regional mean NMB for daily maximum O_3 for the four regions shown in Fig. 6 for the entire 2-year forecast period. The gray stippled areas indicate the Oct.-Mar. cold seasons.

As an example, Figures 7 to 9 show the monthly variation of G-M15 NMB for this period for the four regions for O_3, $PM_{2.5}$, and NO_2, respectively. Several features are worth noting. For one, the seasonal variation in NMB is similar between Year 1 and Year 2 except for $PM_{2.5}$ for Canada (see Sec. 5.2). For another, NMB seasonal variation and magnitude is qualitatively similar for western and eastern Canada for O_3 and $PM_{2.5}$ but is qualitatively different for the western and eastern U.S. regions. O_3 is consistently underpredicted in the western U.S. region but is overpredicted in the warm season and underpredicted in the cold season in the eastern U.S. region. $PM_{2.5}$, on the other hand, is generally underpredicted in the western U.S. and overpredicted in the eastern U.S. in all seasons.

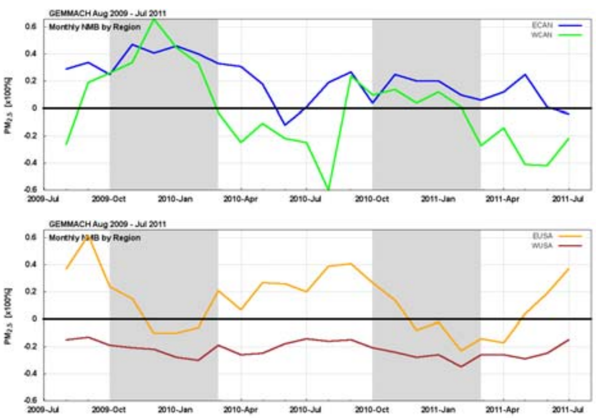

Fig. 8. Same as Fig. 7 but for daily maximum $PM_{2.5}$.

Fig. 9. Same as Fig. 7 but for daily maximum NO_2.

5.4 Diurnal Variation of Model Errors

Figure 10 compares the observed and predicted Canada-mean diurnal variation of hourly O_3, $PM_{2.5}$, and NO_2 concentrations for two seasons, winter (DJF) and summer (JJA). For all three pollutants, the diurnal patterns are distinct for the two seasons for both measurements and model predictions. For O_3 the model tracks the observed diurnal variation quite well but underpredicts in the winter and overpredicts slightly in the summer. For $PM_{2.5}$ the model has a much stronger diurnal variation in the winter than is observed and overpredicts at night, whereas in the summer, it tracks the moderate observed diurnal variation reasonably well and has a smaller bias. And for NO_2 the model tracks the observed bimodal diurnal variation (suggestive of urban "rush hours") quite well in the winter but tends to overpredict nighttime NO_2 levels in the summer.

6. MODEL POST-PROCESSING

After each G-M15 run finishes, hourly fields of O_3, $PM_{2.5}$, and NO_2 are provided to a statistical post-processing package named Updateable Model Output Statistics for Air Quality (UMOS-AQ; see Antonopoulos et al., 2010). For each hour, the UMOS-AQ package applies hour-specific statistical regression equations that have been derived using historical data for each Canadian O_3, $PM_{2.5}$, and NO_2 measurement station and that use model forecast values of O_3, $PM_{2.5}$, and NO_2 plus values of selected G-M15 meteorological parameters plus the previous day's measured concentrations at that hour to forecast hour- and station-specific O_3, $PM_{2.5}$, and NO_2 values. UMOS-AQ has been found to be very successful in removing model biases at locations for which measurements are available.

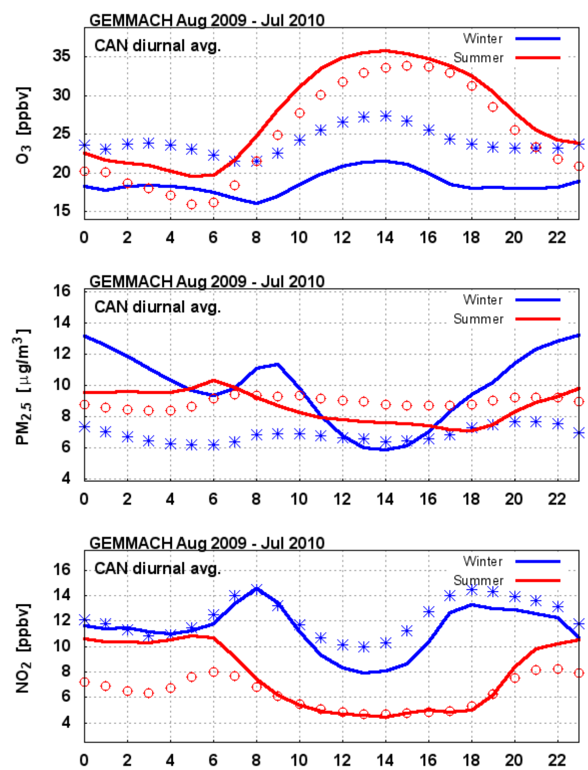

Fig. 10. Diurnal variation of observed and predicted hourly Canada-mean O_3, $PM_{2.5}$, and NO_2 for the winter (DJF) and summer (JJA) seasons. Solid lines denote model values and individual symbols denote observed values.

7. FUTURE PLANS

A new version of GEM-MACH, v1.4.4, is expected to become operational in Oct. 2011. The new version uses an updated version of the GEM model code (v3.3.3) and uses a new set of emissions files that are based on a 2012 U.S. projected emissions inventory instead of the 2005 U.S. national inventory. Given the significant changes in NO_x, VOC, SO_2, and primary $PM_{2.5}$ emissions over the eastern U.S. in the past half decade (e.g., Fioletov et al., 2011), the 2012 projected emissions were expected to be more representative of 2011 U.S. emissions than the 2005-based emissions, and model performance scores have in fact improved when the 2005 U.S. inventory was replaced by the 2012 inventory.

GEM-MACH is also being migrated to a new generation of GEM, version 4. Among the changes introduced in GEMv4 are a switch from an unstaggered to a staggered vertical discretization, a merger of the physics and chemistry "buses" that are used to communicate between the physical and chemical parameterizations and the GEM dynamics kernel, and implementation of upper-boundary "piloting" for nested, limited-area grid configurations such as G-M15. This last feature will have the benefit of allowing fewer vertical levels to be considered, thus reducing execution time. The back-end supercomputers used by the Canadian Meteorological Centre to make meteorological an AQ forecasts will also be upgraded in fall 2011 from IBM air-cooled p5-type machines to water-cooled p7 machines, improving overall execution time by a factor of 2 to 4.

Also, experimental hourly O_3 and $PM_{2.5}$ objective analyses (OAs), which are generated the following day by applying an optimal interpolation scheme to blend G-M15 forecast fields and station measurements, have undergone extensive evaluation and are likely to be added to the G-M15 operational post-processing suite. This will open the door to using these OA fields as part of a model initialization procedure for the next 48-hour G-M15 simulation.

As well, the other member of the post-processing suite, UMOS-AQ, was upgraded in Aug. 2011 to a new version called UMOS-AQ/MIST (Moteur d'Interpolation STatistique), which uses a horizontal interpolation scheme that combines model forecast fields with UMOS-AQ point forecasts to provide point forecasts for Canadian urban locations that lack AQ monitors.

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