

A NEW CANADIAN AIR QUALITY FORECAST MODEL: GEM-MACH15

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1 INTRODUCTION

Operational air quality (AQ) forecasting began in Canada in 2001 with the implementation by Environment Canada (EC) of a continental-scale, 21-km, ozone-only version of the off-line regional CHRONOS (Canadian Hemispheric and Regional Ozone and NO_x System) chemical transport model (Pudykiewicz et al., 1997; Sirois et al., 1999). The meteorological driver used was the regional configuration of EC's operational GEM weather forecast model (Côté et al., 1998a,b). Operational forecasts of PM_{2.5} and PM₁₀ using a simple 2-bin sectional representation followed in 2003.

Work to develop a new EC operational AQ forecast model called GEM-MACH (Global Environmental Multiscale model - Modelling Air quality and CHemistry) started in 2006 (Talbot et al., 2008). A primary motivation for this project was that CHRONOS was not coded so as to be able to run in a massively parallel computing environment, and hence it could not take full advantage of the computer resources of the EC operational weather centre. As a consequence, the model could not be further enhanced without exceeding the limits on timeliness demanded of an operational model.

The project objective was to replace CHRONOS with an on-line chemical transport model, embedded within GEM, that had a superior chemistry package, including a better representation of fine particles. The construction of an on-line model would permit two-way feedbacks between meteorology and chemistry and provide the basis for the future development of a chemical data assimilation system.

Several years of research and development culminated with the implementation in November 2009 of GEM-MACH15, a limited-area 15-km version of GEM-MACH, in place of CHRONOS. As EC's new operational AQ model, GEM-MACH15 is currently integrated twice per day to provide 48-hour guidance for Canada's national AQ forecast program. This paper presents a short description of the chemistry library, the regional configuration, and evaluation results of the new operational model.

2 CHEMISTRY PACKAGE AND EMISSIONS PROCESSING

A number of AQ process representations from EC's AURAMS (A Unified Regional Air-quality Modelling System) chemical transport model (e.g., Gong et al., 2006; Smyth et al., 2009) have been implemented in GEM-MACH, including gas-phase, aqueous-phase, and heterogeneous chemistry and aerosol processes.

Like CHRONOS, GEM-MACH uses a 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 in GEM-MACH and additional processes affecting PM concentrations have been included. CHRONOS considers six chemical components: SO₄, NO₃, NH₄, secondary organic aerosol (SOA), H₂O, and "primary" PM. GEM-MACH considers nine chemical components as it separates the CHRONOS "primary" component into elemental carbon (EC), primary organic aerosol (POA), crustal material (CM), and sea salt (SS).

Both models represent inorganic gas-particle partitioning, PM sedimentation and dry deposition, in-cloud scavenging, and secondary organic aerosol formation (CHRONOS uses the Pandis et al. (1992) SOA scheme whereas GEM-MACH uses the Jiang (2003) scheme). In addition GEM-MACH considers

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sea-salt emissions, aerosol nucleation, condensation, coagulation, and below-cloud scavenging, and aerosol activation and aqueous-phase chemistry. To calculate inter-bin condensational/evaporative transfers, the two bins are subdivided into sub-bins to account better for size dependence. The same approach is used to calculate dry deposition velocities. Table 1 provides a summary of the

chemical process representations employed in GEM-MACH.

The SMOKE emissions processing system is used to produce anthropogenic input emission files on the GEM-MACH rotated latitude-longitude grid based on the 2006 Canadian and 2005 U.S. national inventories. Biogenic emissions are estimated on-line using the BEIS v3.09 algorithms.

PROCESS	DESCRIPTION
PM Composition and Size Distribution	2 size bins: PM _{2.5} , PM ₁₀ 9 chemical species: SO ₄ , NO ₃ , NH ₄ , EC, pOA, sOA, CM, SS, H ₂ O
Emissions	PM _{2.5} and PM ₁₀ emissions speciated to 7 species by primary source type (major point, minor point, area, mobile); 17 gas-phase species emitted
Gas-Phase Chemistry Mechanism	ADOM-II mechanism (Stockwell and Lurmann, 1989): 1) 42 species, 114 rxns; p-SO ₄ replaced by H ₂ SO ₄ + p-SO ₄ 2) N ₂ O ₅ + H ₂ O "heterogeneous nitrate formation" rate enhancement off
Aqueous-Phase Chemistry	ADOM aqueous-phase chemistry (20 species, 20 rxns)
Heterogeneous Chemistry	HETV (Makar et al., 2003), based on ISORROPIA
Aerosol Dynamics	Sedimentation, nucleation, condensation, coagulation, swelling, activation, (S. Gong et al., 2003)
Secondary Organic Yields	IAY scheme based on Jiang (2003, 2004); 5 lumped VOC species form SOA
Dry Deposition	Zhang et al. (2001) scheme (land-cover- and size-dependent)
Wet Deposition	Transfer of tracers from cloud to rain water based on precipitation production. In-cloud and below-cloud scavenging of soluble gases and particles (size-dependent) (W. Gong et al., 2006).
Chemical Boundary Conditions	Climatological profiles with Davies lateral boundary conditions

Table 1. PM chemical and physical process representations in GEM-MACH.

3 OPERATIONAL CONFIGURATION

GEM-MACH15, a limited-area forecast configuration of GEM-MACH, uses a continental-scale domain with 15-km horizontal grid spacing on a 348x465 rotated latitude-longitude grid. The 58 vertical levels extend from the surface to 0.1 hPa on a hybrid vertical coordinate. Time-dependent meteorological lateral boundary conditions (LBCs) are provided by GEM15, the EC operational weather forecast model used for regional two-day forecasts. GEM15 is a variable-resolution global model that has a uniform-resolution core domain of 15-km grid spacing centred over North America. Monthly-average concentration vertical profiles for different species are used to provide chemical LBCs. The chemistry fields are initialized by cycling the 12-h forecast of the previous model run.

The precise placement of the GEM-MACH15 domain over North America was in part dependent upon the existing location of the core sub-domain of GEM15. In order to avoid the need for interpolation of

the initial and boundary conditions provided by GEM15, the grid points of the GEM-MACH15 grid were chosen to be co-located with those of GEM15 (Figure 1). A comparison of the position of the GEM-MACH15 grid with that of CHRONOS indicates improved coverage over the Arctic regions of Canada, and slightly less coverage of the extreme southern U.S. and northern Mexico (Figure 2).

Table 2 provides a short summary of the differences between the operational configurations of CHRONOS and GEM-MACH15. The time step for the integration of the chemical processes has been substantially reduced for the new model (from 1 hr to 15 mins). The meteorology in GEM-MACH15 is integrated with a time step of 7.5 mins, the same time step used for GEM15. After tests confirmed there would be no significant degradation in the chemical forecasts, it was decided to integrate the chemistry every second time step (i.e., 15 mins) in order to reduce the run time of the new model.

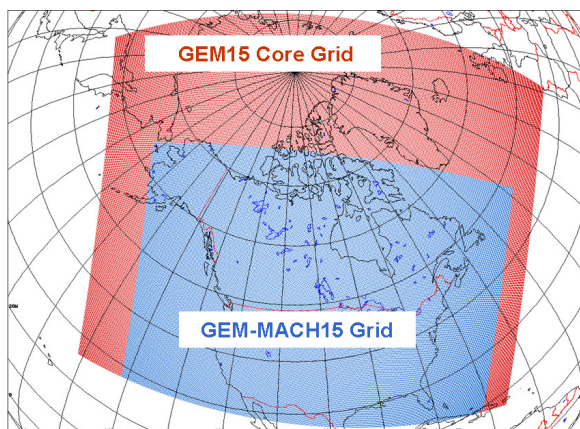


Figure 1. The GEM-MACH15 grid is a subgrid of and is co-located with points of the uniform core grid of GEM15.

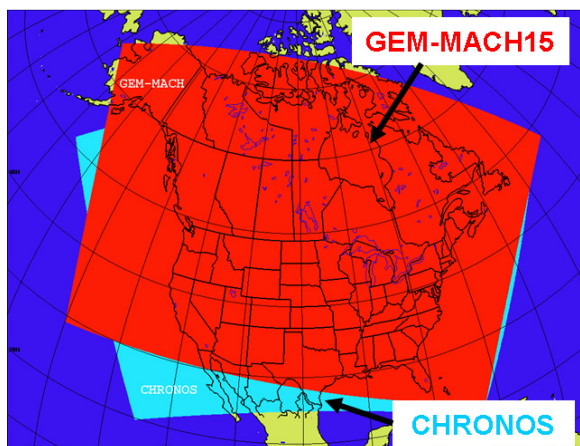


Figure 2. Comparing grid coverage of GEM-MACH15 to that of CHRONOS.

	CHRONOS	GEM-MACH15
Grid projection	Polar Stereographic	Rotated Lat-Lon
Grid configuration	Limited area (LU)	Limited Area (LU)
Model horizontal resolution	350x200 (Dx=21 km)	348x465 (Dx=15 km)
Model time step	3600 s (Chemistry)	450 s (Meteorology), 900 s (Chemistry)
Model top	24 Gal-Chen levels up to 6 km	58 Hybrid levels up to 0.1 hPa (~60 km)

Table 2. A comparison of the operational configurations for CHRONOS and GEM-MACH15.

4 MODEL EVALUATION

Prior to operational implementation, GEM-MACH15 was evaluated for two periods during the winter and summer seasons of 2008. The winter evaluation period went from February 14 to March 22, 2008 after a two-week spin-up period and the summer

evaluation period went from June 19 to July 26, 2008, again with a two-week spin-up period.

A comparison of the mean 20-h forecast fields for ozone and PM_{2.5} for each evaluation period for the runs initialized at 00 UTC of the two models provides a general indication of the main differences in model forecasts. For ozone (Figure 3), we see that in the summer the forecasts from GEM-MACH15 are slightly higher for most urban centres, while larger differences are observed in remote areas of the domain. This is due to the use of a different set of chemical LBCs for GEM-MACH15 (Dirichlet) vs. CHRONOS (Neumann), which provide GEM-MACH15 with more realistic background levels for ozone. As expected, the impact is much greater in the winter season, since ozone production is substantially reduced in urban centres and chemical LBCs play a larger role.

For PM_{2.5} (Figure 4), in the summer GEM-MACH15 predicts higher mean concentrations than CHRONOS, particularly in the eastern region of the domain, whereas in the winter the new model forecasts lower concentrations than CHRONOS. These differences are due in part to different vertical diffusion schemes used by the two models, to the lack of aqueous-phase chemistry in CHRONOS, and to the use of newer emissions inventories by GEM-MACH15.

Table 3 gives a summary of evaluation statistics for GEM-MACH15 and CHRONOS for both summer and winter seasons. These scores were computed using hourly observations of ozone and PM_{2.5} obtained in near real-time from the AIRNow network for U.S. observation stations (see <http://airnow.gov>) and from the regional data providers for Canadian stations. A dramatic reduction in mean bias for ozone from GEM-MACH15 in the winter season follows what is observed in Figure 3. For PM_{2.5}, CHRONOS has a negative bias in the summer vs. a weak positive bias for GEM-MACH15. The reverse occurs for the winter: a weak positive bias for CHRONOS vs. a weak negative bias for GEM-MACH15.

In terms of the correlation coefficient and the unbiased RMSE, GEM-MACH15 shows modest improvements for ozone and somewhat mixed results for PM_{2.5}. The decision to proceed with the operational implementation of GEM-MACH15 was supported by evidence that overall the new model's performance was equal to or slightly better than CHRONOS together with a far better potential for performance improvements in the future following further model development.

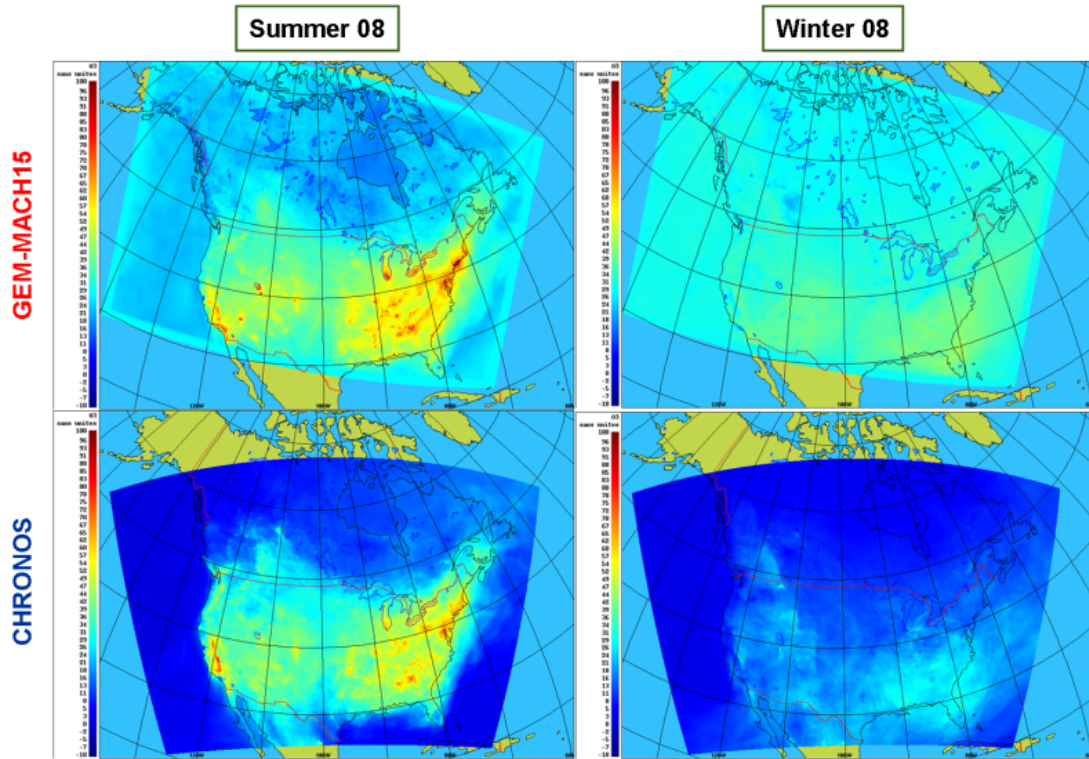


Figure 3. Mean 20 UTC ozone field (ppbv) for the summer (left) and winter (right) periods predicted by CHRONOS (bottom) and GEM-MACH15 (top) after 20 h of simulation beginning at 00 UTC.

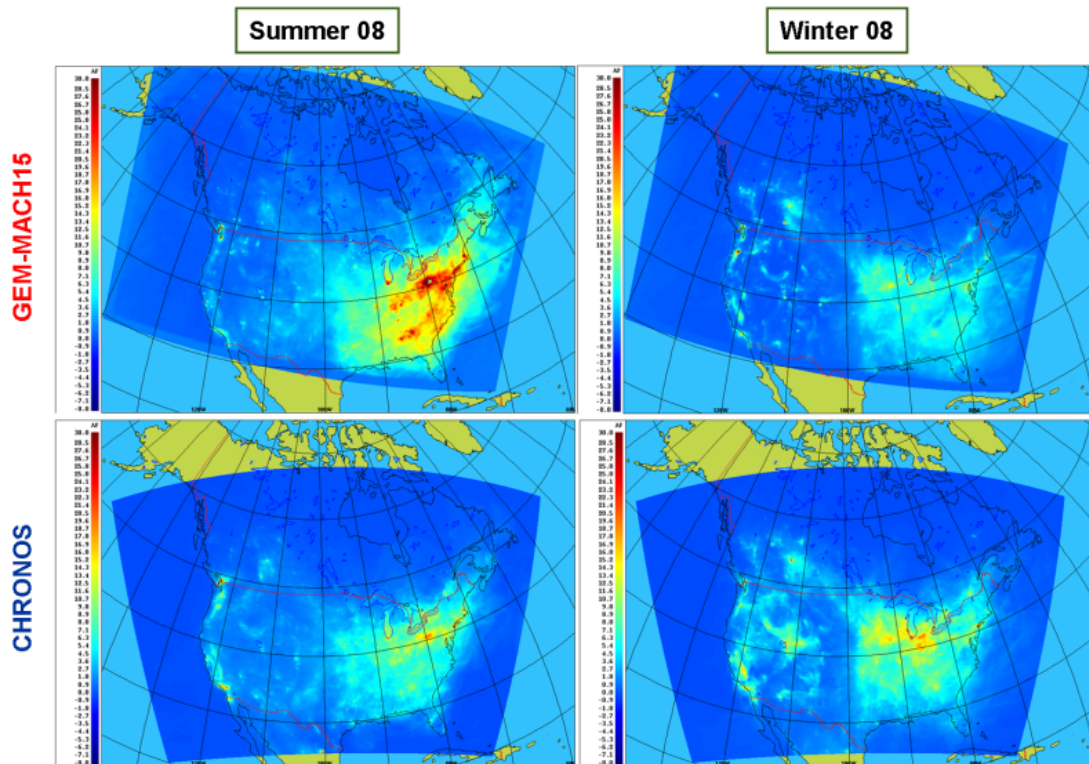


Figure 4. Mean 20 UTC $PM_{2.5}$ field ($\mu g m^{-3}$) for the summer (left) and winter (right) periods predicted by CHRONOS (bottom) and GEM-MACH15 (top) after 20 h of simulation beginning at 00 UTC

Summer 2008				
Metric	Hourly O ₃ (ppbv)		Hourly PM _{2.5} (µg m ⁻³)	
	CHRONOS	GEM-MACH15	CHRONOS	GEM-MACH15
R	0.68	0.68	0.30	0.40
MB	-4.31	2.52	-2.08	0.69
RMSE unbiased	15.39	15.33	12.77	13.48
Winter 2008				
Metric	Hourly O ₃ (ppbv)		Hourly PM _{2.5} (µg m ⁻³)	
	CHRONOS	GEM-MACH15	CHRONOS	GEM-MACH15
R	0.46	0.58	0.26	0.22
MB	-19.48	-5.49	0.86	-0.18
RMSE unbiased	12.77	12.15	14.11	15.93

Table 3. Objective scores (correlation coefficient, mean bias, and RMSE after bias is removed) for CHRONOS and GEM-MACH15 for 48-h forecasts (all hours) for the summer and winter periods of 2008.

5 SUMMARY

In November 2009, Environment Canada implemented a new operational AQ forecast model called GEM-MACH15 to support its year-round national forecast program. This model includes a more sophisticated chemical process package than was available for the previous model, CHRONOS, particularly with respect to the treatment of fine particles. GEM-MACH15 is an on-line chemical transport model embedded within EC's operational GEM weather forecast model. This opens the door in the future to be able to represent two-way feedback processes between meteorology and chemistry, and also creates a platform more suitable for chemical data assimilation.

Evaluation of the model over summer and winter periods in 2008 indicate that the new model in general performs better than CHRONOS for ozone and PM_{2.5} in summer and for ozone in winter, though with a slight deterioration for PM_{2.5} in winter. Updates to the new model are planned at yearly intervals following a standard research-to-development-to-operations approach.

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