# FROM THE PACIFIC TO THE ATLANTIC:
# MODELS-3 PERFORMANCE IN COASTAL AREAS OF CANADA

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## 1. INTRODUCTION

Over the past five years, the authors have been using Models-3 to study regional smog in coastal areas of western and eastern Canada. In this paper, we compare and contrast the modelling strategies adopted, and make selected comparisons of findings from the various studies.

In western Canada, studies have focused on the Lower Fraser Valley (LFV), where the City of Vancouver is located (population of over 2 million). Not far to the south of the LFV lies Seattle, Washington, a city of comparable size. The LFV airshed is confined by the presence of large mountains to the north and south, and coastal areas to the west, and is subject to relatively little long-range transport of pollutants. The isolated nature of the airshed, the climate of the region, and aggressive air quality management over the past two decades have resulted in lower levels of smog than other similarly populated regions of Canada. However, ongoing improvement to the understanding and management of smog in the area is needed.

Studies conducted by the authors for the LFV have been aimed at examining the potential for trans-boundary pollutant transport between Canada and U.S. (e.g., Di Cenzo and Lepage, 2003), the effects of anticipated future changes in emissions in the region, and the effects of alternative fuels for passenger vehicles on regional air quality (Lepage and Van Altena, 2001; Vitale *et al.*, 2004).

In eastern Canada, studies have covered southern Ontario (which has significant coastal area bordering the Great Lakes), southern Quebec, and the Maritime provinces. Wind flows in these areas of the country are unlike the LFV, and long-range transport of pollutants from one region to another and from upwind regions in the northeast United States is a significant contributor to smog levels. Long-range transport and trans-boundary effects have been a key focus of these studies. The effects of committed and hypothetical emission reduction strategies in Canada and the US have been examined, as well as the role of major point sources on regional smog (Lepage *et al.*, 2002).

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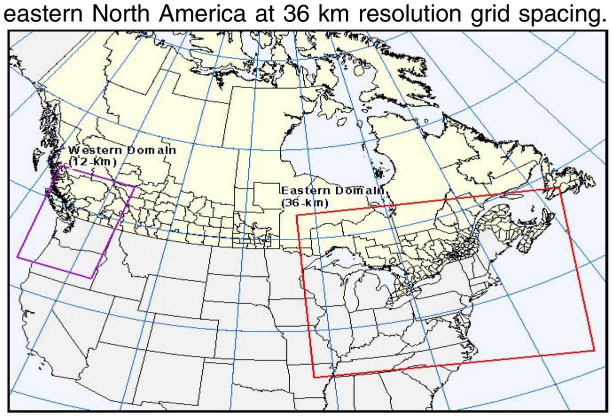
## 2. MODELLING METHODOLOGY

### 2.1 *Photochemical model*

The modelling described in this paper was conducted using the U.S. EPA's Community Multi-scale Air Quality (CMAQ) model. In the most recent work, version 4.3 of CMAQ was used. The RADM2 and CB-IV chemical mechanisms were used to model the LFV and Eastern Canada, respectively. Recently, the SAPRC99 chemical mechanism has been adopted for on-going modelling of the LFV and Eastern Canada. The authors have also been working with researchers at the University of California, Riverside, to implement a version of SAPRC99 and CMAQ that treats 1,3-butadiene and benzene explicitly (Carter, 2004).

### 2.2 *Model Domains and Grid Spacings*

Figure 1 shows the primary model domains. In eastern Canada, the desire to examine long-range transport has dictated a large model domain that covers much of eastern North America at 36 km resolution grid spacing.




Limited studies have also been performed on sub-regions with grid spacings of 12 and 4 km.

**Figure 1.** CMAQ Model Domains.

In the LFV, long-range transport is minimal, allowing for a smaller model domain. However, the mountainous topography requires greater horizontal and vertical resolutions to resolve diurnal wind flow patterns. A model domain with a grid spacing of 12 km, and a sub-domain with a grid spacing of 4 km have been used.

Fifteen vertical levels define the vertical structure for the CMAQ runs: the lowest being ~40 m above the surface, the highest at ~15,000 m, and 10 layers in the lowest 3000 m.

### 2.3 *Meteorological Fields*

CMAQ requires 3-dimensional meteorological data as input. For eastern Canada, the authors ran the MM5 mesoscale meteorological model on a North American-wide domain with a grid spacing of 108 km, and then on sub-domains with grid spacings of 36 km, 12 km and 4 km. In all cases, the MM5 modelling had 30 vertical levels, with 17 levels in the lowest 3000 m.

For the LFV, we relied on meteorological modelling performed by the University of British Columbia, at a horizontal grid spacing of 4 km, using the MC2 mesoscale model. UBC runs MC2 in a forecast mode, on a daily basis. To accommodate the MC2 output data in CMAQ, the authors developed conversion software to interpolate the MC2 data, which are in a polar-stereographic map projection to the required Lambert conical-conformal projection at grid spacings of 4 km and 12 km (Qiu *et al.*, 2004). The conversion software also transposes the data from the MC2 variable set to the MM5 variable set, and converts from the MC2 to the MM5 data formats in preparation for input to MCIP. The MC2 data were provided on 38 vertical levels, with the lowest level at 130 m above the surface and the highest at 18,000 m. In the process of converting to MM5 format, MC2 results were interpolated to 30 vertical levels, ranging from approximately 40 m to 16,000 m.

### 2.4 *Emission Inventories*

Emission inventory data for Canada and the US were prepared using the Sparse Matrix Operator Kernel Emission processing system (SMOKE, version 2.0).

The most recent emission inventory data available were used which, for Eastern Canada, consisted of the Canadian national inventory of Common Air Contaminants (CAC) for the year 1995, produced by Environment Canada, and the U.S. National Emission Inventory (NEI, version 2.0) for the year 1999. For the LFV, the Greater Vancouver Regional District's emission inventory for the year 2000 was adapted for use in SMOKE, along with the 1995 CAC inventory and the 1999 NEI for portions of the study domain that are outside the LFV. Biogenic emissions in both eastern and western Canada were developed using the BEIS model, with the most recent work based on BEIS3.

### 2.5 *Model Episodes*

In Eastern Canada, three historical smog events have been examined: July, 1999; August, 2001; and February, 1998. For the LFV, the month of August, 2001 has been modelled. This period coincided with the Pacific 2001 field monitoring campaign, which entailed surface-based and aircraft measurements of various pollutant species and meteorological measurements. The first half of December, 2002 has also been modelled. This period included relatively cool temperatures typically associated with elevated levels of airborne particulate matter due to wood-fired space heating and other combustion sources.

## 3. SELECTED RESULTS

### 3.1 *Ground-Level Ozone in the LFV*

Model performance for the period from August 9 to August 20, 2001 in the LFV was evaluated against air quality monitoring data at several locations for both the 4 km grid spacing and 12 km grid spacing outputs, keeping in mind that, in both cases. In general, the 4 km grid spacing offered relatively little improvement over the 12 km gird spacing in predicting hourly concentrations of ground-level ozone and $PM_{2.5}$.

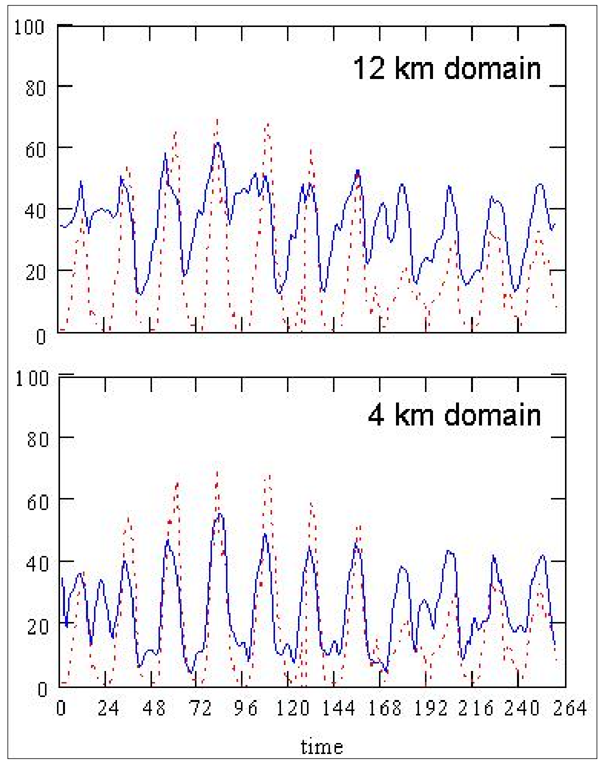



**Figure 2.** Modelled (dashed) and measured (solid) time history of ozone concentrations at Pitt Meadows for: a) 12 km domain, and b) 4 km domain.

Figure 2 shows an example of model performance for ground-level ozone, at a location in the eastern suburbs of Vancouver, near the north slopes of the LFV (Pitt Meadows). At the 12 km grid spacing (Figure 2a), CMAQ provided reasonably good predictions of daytime peak ozone levels, but significantly overestimated nighttime concentrations. At a 4 km grid spacing (Figure 2b), the prediction of daytime peak ozone levels was not much altered, but the nighttime ozone predictions were greatly improved. This may have been due to the fact that, among other things, nighttime ground-level ozone is highly sensitive to the distribution of $NO_X$ emissions, which were better resolved on the 4 km grid. At locations further inland, where the valley is narrower, the degree of improvement in nighttime ozone levels was more modest, indicating the need for finer horizontal and/or vertical resolutions to better reproduce evening $NO_X$ concentrations and the overnight titration of ozone.

The August 9 to 20, 2001 period had two distinct meteorological phases: a dry, stagnant period followed by a cooler, well mixed phase with extensive marine cloud penetrating into the valley. During the stagnant phase, the model consistently underestimated daytime peak ozone levels (Figure 2). When the model indicated that ozone levels were beginning to decline, the observed concentrations often continued to rise to a peak in the late afternoon. This occurred at a time when the wind flows were beginning to transition from daytime sea breeze and up-slope flows to nighttime land breeze and down-slope flows. We speculate that vertical recirculations associated with these flows lead to the transport of ozone from the top of the boundary layer to the surface, and that this effect occurred at a scale that was not resolved by the meteorological model. Similar effects have been observed in areas of southwestern Ontario affected by lake breezes (Hopper, 2004).

During the well-mixed phase (the last several days of the simulation), the model consistently overestimated daytime peak ozone concentrations. The extensive cloud cover and cooler temperatures during this phase did not favour the formation of ground-level ozone and observed concentrations were generally much lower than during the stagnant phase, although predicted levels were only slightly lower. An evaluation of the MC2 meteorological modelling (Snyder, 2003) indicated that the model overestimated boundary-layer temperatures in the LFV during the well-mixed phase, which may have caused the overestimate of modelled ground-level ozone.

### 3.2 *PM2.5 in the LFV*

Figure 3 shows an example of model performance for $PM_{2.5}$ (12 km grid) at a location in the eastern part of downtown Vancouver (Slocan Park). The model failed to reproduce the observed pattern of hourly variations in PM levels, but did a reasonably good job of reproducing the 24-hour average on most days. This was generally the case at all monitoring sites in the LFV. This is helpful in that ambient air quality guidelines for $PM_{2.5}$ are based on 24-hour averages. Modelled hourly concentrations showed a strong diurnal trend with early morning peaks, which did not exist in the observations.

The monitoring site at Slocan Park also offered us an opportunity to examine data for individual components of the $PM_{2.5}$, including nitrates, sulfates, ammonium and total organic PM. Examining these data (not shown here), we found that hourly sulfate concentrations were reproduced extremely well by the model, and hourly total organic PM was reproduced reasonably well, although with a stronger diurnal fluctuation than actually occurred. The hourly nitrate and ammonium levels were not reproduced well, and it was for these compounds that the spurious early morning peak was particularly strong.

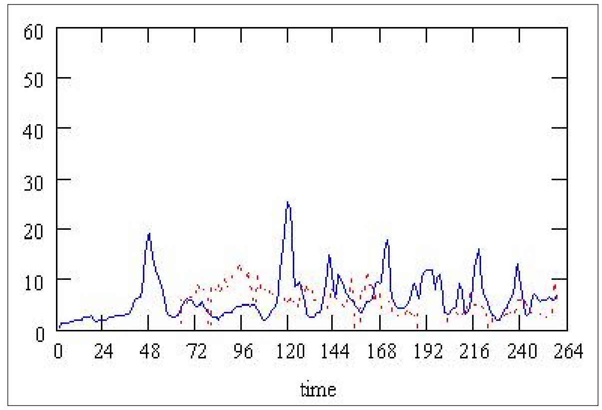



**Figure 3.** Modelled (dashed) and measured (solid) time history of $PM_{2.5}$ concentrations (μg/$m^3$) at Slocan.

Zhang *et al.* (2003) noted similar problems with nitrate predictions from CMAQ simulations for the eastern U.S. They attributed the spurious peaks to errors in nitrate aerosol activity coefficients under certain conditions.

### 3.2 *Ozone and $PM_{2.5}$ in Eastern Canada*

The performance of CMAQ for eastern Canada was evaluated for the period from July 11 to July 19, 1999. This period was dominated by southerly to westerly wind flows, with clear skies. Daytime temperatures ramped up from July 11 to 17, as did concentrations of ground-level ozone and PM. By July 18, a cold front moved through the area, bringing northwesterly wind flows, and pollutant concentrations dropped off dramatically.

Figure 4 shows the average model performance for ground-level ozone, for monitoring sites in southern Ontario. As in the LFV, the prediction of daytime peak ozone levels was generally reasonably good, but nighttime ozone levels were overestimated. Increasing the horizontal resolution to 4 km (not shown) produced only a small improvement in nighttime levels. Examination of the model performance for $NO_X$ (not shown) indicated that the model underestimated late evening peaks in $NO_X$, which would lead to an underestimate of overnight titration of ozone by $NO_X$.

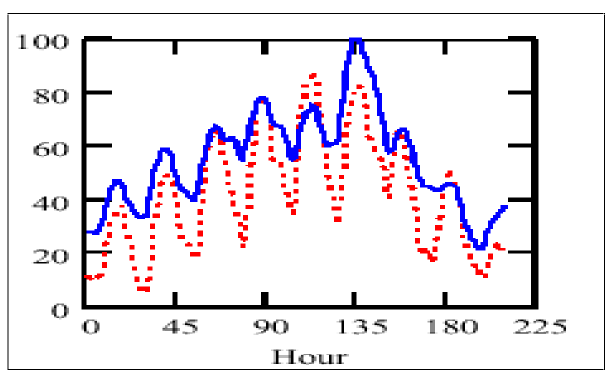



**Figure 4.** Southern Ontario average modelled (dashed) and measured (solid) time history of hourly ozone (ppb) concentrations, July 11-19, 1999.

Figure 5 shows average model performance for $PM_{2.5}$, for monitoring sites in southern Ontario. As with ozone, the general trends are reproduced reasonably well. Although the maximum concentration at the peak of the event is predicted well, the timing and duration of the event is off (i.e., a day late and one day too short). This is likely related to uncertainties in the MM5 predicted rate of passage of the frontal system.

The $PM_{2.5}$ during the July 1999 smog event in eastern Canada was dominated by sulfate aerosol. In the observed data, the sulfate content ranged from 50 to 70%; in the modelled data, the sulfate content was greater (70 to 80%), at the expense of secondary organic aerosol and primary PM. The nitrate content was small, and the problem of spurious nitrate peaks that was observed in the LFV was not observed here.

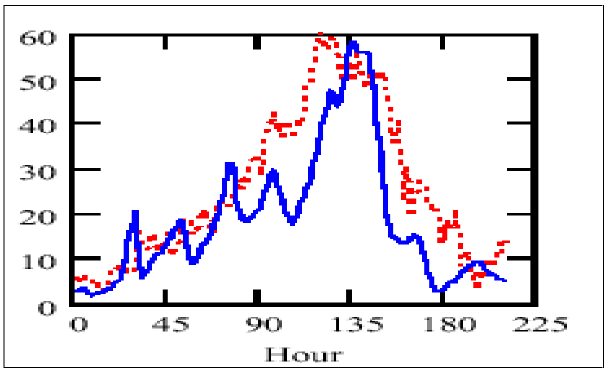



**Figure 5.** Southern Ontario average modellked (dashed) and measured (solid) time history of hourly $PM_{2.5}$ (µg/m3) concentrations, July 11-19, 1999.

### 3.3 *Interesting Results: Electric Vehicle Scenario*

Model runs were performed to examine the effect of widespread introduction of electric passenger vehicles as a replacement for gasoline-powered vehicles in the LFV. Emissions of $NO_X$, VOCs and other exhaust pollutants were reduced, and emissions from electricity generation were increased. A scenario, in which 75% of the gasoline passenger vehicles were replaced with electric vehicles produced only modest reductions in regional emissions of $NO_X$ and VOCs (10 to 15 %).

Figure 6 shows a plot of the change in maximum 24-hour $PM_{2.5}$ resulting from this scenario for the August 2001 modelling period, divided into three sub-regions. The westernmost sub-region represents the Vancouver urban area, the easternmost represents rural areas typically downwind of the urban area during the daytime, and the middle, which represents a transitional zone.

n the transitional and rural areas, we see a general decrease in $PM_{2.5}$ (as high as 13%) as a result of the 75% electric vehicle scenario. In these areas, the reductions in $NO_X$ and VOCs produced corresponding reductions in nitrate and secondary organic aerosol. In much of the urban area, however, $PM_{2.5}$ levels experienced a small increase (up to 2%), primarily related to increases in $NO_X$ emissions from the extra electricity generation needed to power the electric vehicles. For the scenario shown in Figure 6, the extra electricity generation came partly from increased production at the existing Burrard power plant (a gas-fired plant located near downtown Vancouver) and partly from increased hydroelectric production.

Also, at locations where there was a net decrease in $NO_X$ and VOCs, airborne radicals that formerly reacted with these compounds became free to react with $SO_2$, causing a small increase in sulfate aerosol. The latter effect contributed to the non-linearity between emissions and the secondary components of $PM_{2.5}$, and is just one of the many challenges faced in predicting how emission reduction strategies will affect PM.

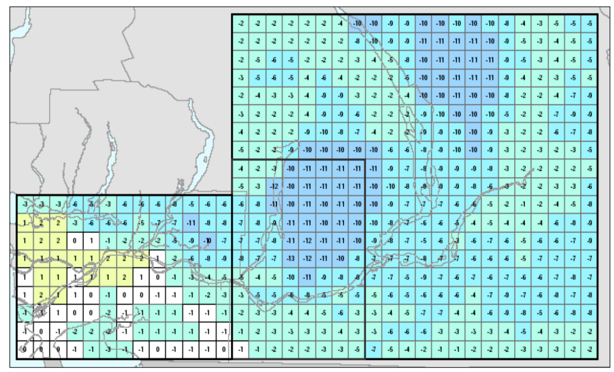


**Figure 6.** Percentage change in modelled 24-hour $PM_{2.5}$ concentrations due to electric vehicles.

## 4. CONCLUSIONS

The authors have undertaken regional photochemical modelling in Canada, using the CMAQ model. This work has shed light on various aspects of model performance, many of which have been identified by other researchers in other jurisdictions. This includes overestimation of nighttime ozone, which appears to be related to insufficient horizontal and/or vertical resolution. It also includes potential underestimation of afternoon peak ozone in areas affected by local wind flow systems, such as sea breezes or valley flows. Spurious predicted nighttime peaks in nitrate aerosol were also predicted by CMAQ, a phenomenon observed by other researchers. Overall, the model performance has been encouraging thus far, with reasonable performance for predictions of daytime peak ozone concentrations and 24-hour averaged $PM_{2.5}$.

## 5. ACKNOWLEDGEMENTS

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