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FROM THE PACIFIC TO THE ATLANTIC: MESOSCALE AIR QUALITY MODELLING IN COASTAL AREAS OF CANADA

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1. INTRODUCTION

Over the past five years, the authors have been using Eulerian photochemical modeling to study regional smog in coastal areas of western and eastern Canada.

In western Canada, studies have focused on the Lower Fraser Valley (LFV), where the City of Vancouver is located, with its population of over 2 million. Not far to the south of the LFV, lies Seattle, a U.S. city of a size comparable to Vancouver. 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 combined to produce lower levels of smog pollutants than in other comparable population centers of Canada. Nevertheless, ongoing management and improved understanding of smog patterns in the airshed are 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., DiCenzo and Lepage, 2003), the effects of anticipated future changes in pollutant emissions in the region, and the effects of alternative passenger vehicles and fuels (electric vehicles and ethanol-blended gasoline) 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, and also southern Quebec and the Maritime provinces. Wind flows in these areas of the country are generally not constrained by large mountains and, unlike the LFV, 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 pollutants. The long-range transport and trans-boundary effects have been a key focus of these studies. The future effects of committed and hypothetical emission reduction strategies both in Canada and the US have also been examined, as well as the role of major point sources (thermal power plants) on regional smog in southern Ontario (Lepage *et al.*, 2002).

In this paper, we compare and contrast the modeling strategies adopted, and make selected comparisons of findings from the various studies.

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2. MODELLING METHODOLOGY

2.1 *Photochemical model*

All of the modeling described in this paper was conducted using the U.S. EPA's Community Multi-scale Air Quality model (CMAQ). This is an Eulerian photochemical model that numerically predicts the transport, diffusion and chemical transformation of air pollutants over a 3-dimensional model grid.

In the most recent work, version 4.3 of CMAQ has been used. This version of the model offers a number of options for the chemical mechanism that is used to simulate the numerous chemical transformations that can take place among pollutants in the atmosphere. The RADM2 chemical mechanism was used to model the LFV and the CB-IV mechanism was used for Eastern Canada. Recently, the authors have adopted the SAPRC99 chemical mechanism for on-going modeling of the LFV and Eastern Canada, and have been working with researchers at the University of California, Riverside, to implement a version of SAPRC99 and CMAQ that treats selected air toxics (1,3-butadiene and benzene) associated with motor vehicle exhausts (Carter, 2004) explicitly.

2.2 *Model Domains and Grid Spacings*

Figure 1 shows the 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. To maintain practical computational requirements, the horizontal grid spacing has generally been kept relatively large, at 36 km. Limited studies have been performed on sub-regions of the domain with grid spacings of 12 km and 4 km, with the intent of taking a more focused look at lake breeze effects in southwestern Ontario.

In the LFV, where long-range transport is minimal, the size of the model domain is much smaller. In this case, however, the mountainous topography of the area requires greater horizontal and vertical resolution to resolve the complexities of the diurnal wind flow patterns in the surface boundary layer. Consequently, a model domain with a grid spacing of 12 km, and a sub-domain (not shown) with a grid spacing of 4 km have been used.

The vertical resolution has been approximately the same in all CMAQ runs for both eastern Canada and the LFV. Fifteen vertical levels were adopted, with the lowest at approximately 40 m above the surface, the highest at about 15,000 m above the surface, and approximately 10 layers in the lowest 3000 m.

Figure 1. LFV and Eastern Canada CMAQ Model Domains.

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 modeling had 30 vertical levels, with 17 levels in the lowest 3000 m (i.e., approx. twice the vertical resolution of the CMAQ runs).

For the LFV, we relied on meteorological modeling 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 continual 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 project and 3.3 km grid spacing, to the required Lambert conical-conformal projection at grid spacings of 4 km and 12 km (Qiu *et al.*, 2004). The software also transposes the data from the MC2 variable set to the MM5 variable set, and converts from the MC2 to the MM5 data format, which can then be input to the MCIP meteorological pre-processor for CMAQ. 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, the data 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 model transforms annual county-wide emission inventory data into gridded hourly emissions at the desired grid-spacings for CMAQ. 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 representative historical periods associated with smog events have been examined: July, 1999; August, 2001; and February, 1998. For the LFV, the month of August, 2001 has been modeled. This period coincided with the Pacific 2001 field monitoring campaign, which entailed surface-based and aircraft measurements of various pollutant species as well as detailed meteorological measurements. The first half of December, 2002 has also been modeled. This period included a stagnant phase with 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 throughout the valley. This was done for both the 4 km grid spacing and the 12 km grid spacing, keeping in mind that, in both cases, the meteorological data used in the model run were interpolated from a 4 km grid spacing. 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 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 generally provided reasonably good predictions of daytime peak ozone concentrations, but significantly overestimated nighttime ozone levels. At the 4 km grid spacing (Figure 2b), the prediction of daytime peak ozone levels was not greatly 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 much more modest, signifying the need for still finer horizontal and/or vertical resolution to better reproduce elevated evening NO_X concentrations that subsequently lead to 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 had a consistent tendency to underestimate daytime peak ozone levels (Figure 2). When the model suggested that ozone levels were beginning to decline, the observed concentrations often continued to rise to a brief peak in the late afternoon or early evening. 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 transport of ozone from the top of the boundary layer to the surface, and that this effect occurred at a scale that was not adequately resolved by the meteorological modeling. 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. Predicted concentrations, on the other hand, were only slightly lower. An evaluation of the MC2 meteorological modeling (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 modeled ground-level ozone.

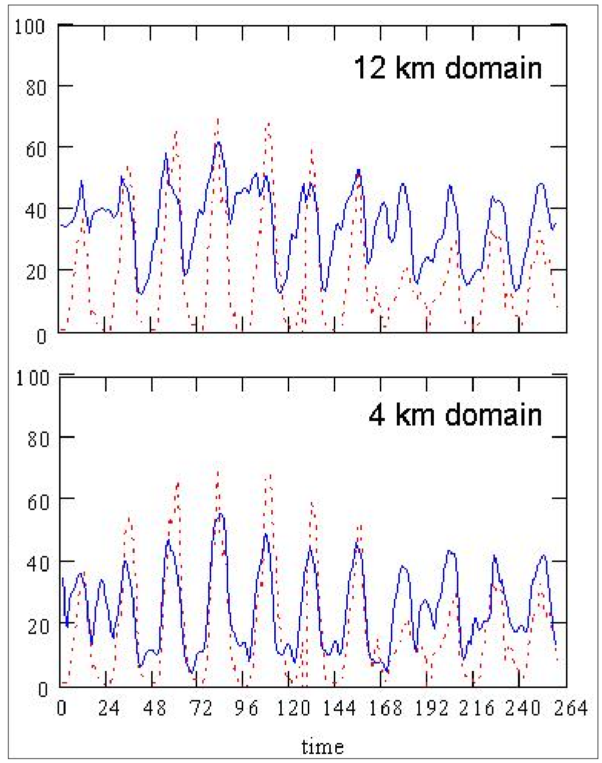

Figure 2. Modeled (dashed) and measured (solid) time history of ozone concentrations at Pitt Meadows for: a) 12 km domain, and b) 4 km domain.

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 figure shows that 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 concentration on most days. This was generally the case at all monitoring sites in the LFV. The latter finding, at least, is helpful since 24 hours is a relevant averaging time in terms of ambient air quality guidelines for $PM_{2.5}$. The modeled hourly concentrations showed a strong diurnal variation (with early morning peaks), which did not exist in the actual observations.

The monitoring site at Slocan Park 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. 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.

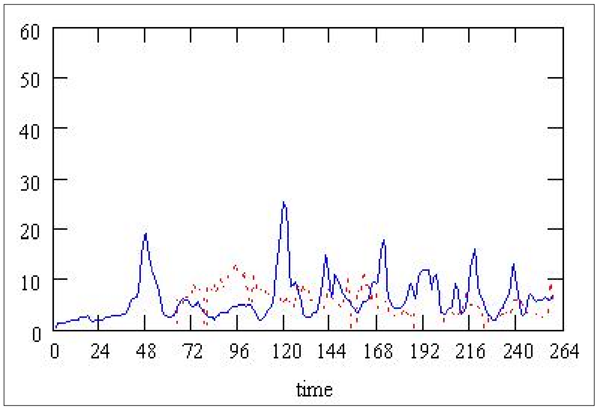

Figure 3. Modeled (dashed) and measured (solid) time history of $PM_{2.5}$ concentrations ($\mu g/m^3$) at Slocan,12 km domain.

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

Performance of the CMAQ modeling 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 (36 km grid). As in the LFV, the prediction of daytime peak ozone levels was generally reasonably good, but nighttime ozone levels were substantially overestimated. Increasing the horizontal resolution to 4 km (not shown) produced a small improvement in the nighttime levels. Examination of the model performance for NO_X (not shown) indicated that the model significantly underestimated late evening peaks in NO_X concentrations, which would lead to an underestimate of overnight titration of ozone by NO_X. This was most likely caused by insufficient vertical resolution to simulate the very limited vertical diffusion that occurs during nighttime inversions.

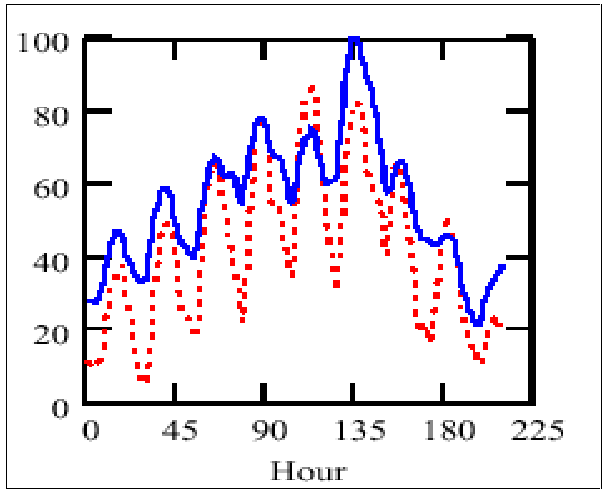

Figure 4. Southern Ontario average modeled (dashed) and measured (solid) time history of hourly ozone (ppb) concentrations, July 11-19, 1999.

Figure 5 shows average model performance for $PM_{2.5}$, for monitoring sites in southern Ontario. As with ground-level ozone, the general trend of increasing concentration over the period from July 11 through July 17 is reproduced reasonably well. Although the maximum concentration at the peak of the event is predicted well, the timing of the event is off. The period when concentrations exceeded 30 $\mu g/m^3$ was predicted to span about 1.5 days when in reality, it spanned about 2.5 days. The predicted event arrived late in southern Ontario and passed through the area too quickly. This is undoubtedly related to uncertainties in the MM5 meteorological modeling and the predicted rate of passage of the frontal system through the area.

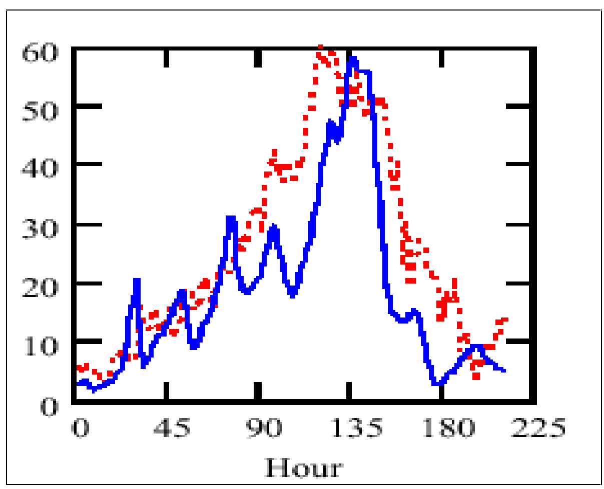

Figure 5. Southern Ontario average modeled (dashed) and measured (solid) time history of hourly $PM_{2.5}$ ($\mu g/m^3$) concentrations, July 11-19, 1999.

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 was in the range from 50 to 70%; whereas, in the modeled data, the sulfate content was greater, in the range from 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.

3.3 *Interesting Results: Electric Vehicle Scenario*

A series of model runs was performed to examine the effect of widespread introduction of electric vehicles as a replacement for gasoline-powered passenger vehicles in the LFV. Under this scenario, emissions of NO_X, VOCs and other motor vehicle exhaust pollutants were greatly reduced, and emissions from electricity generation were increased somewhat. 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 %) from all sources.

In the transitional and rural areas, we see a general decrease in PM2.5 (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, the $PM_{2.5}$ levels experienced a small increase (up to 2%). This was primarily related to an increase in NO_X emissions from the extra electricity generation needed to power 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.

We also found that, at locations where there was a net decrease in NO_X and VOC's, airborne radicals that formerly reacted with these compounds became free to react with SO_2, causing a small, partially offsetting increase in sulfate aerosol. The latter effect contributed to the non-linearity of the relationships 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.

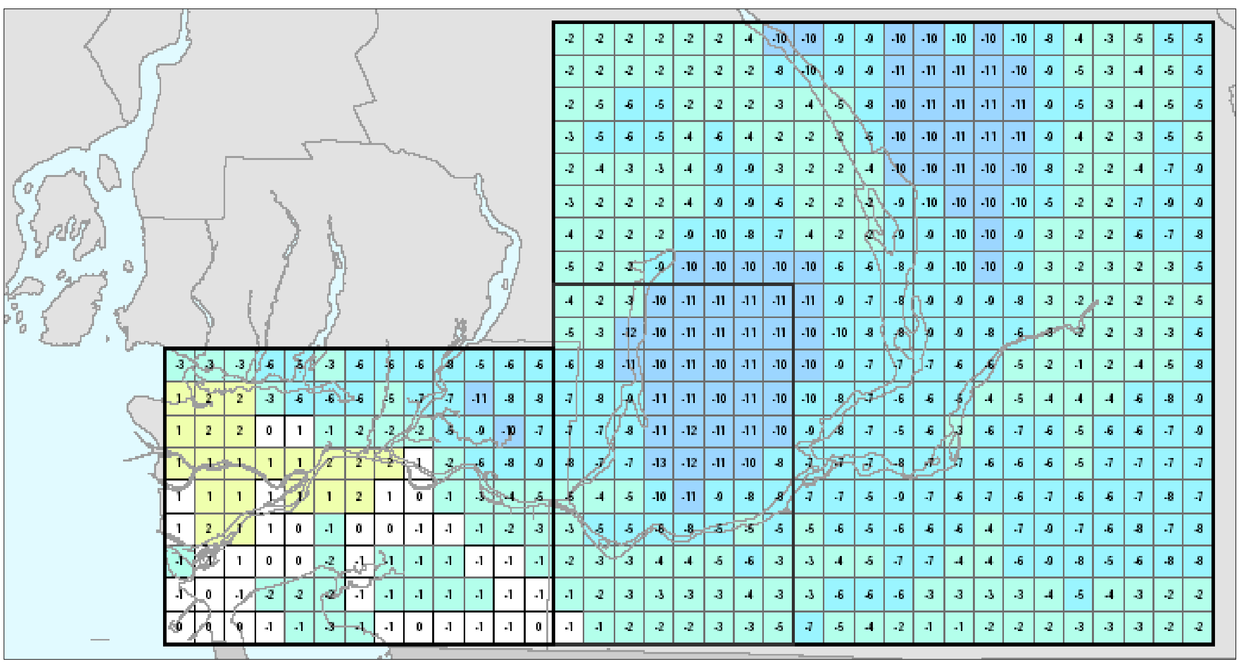

Figure 1. Percentage change in modeled 24-hour $PM_{2.5}$ concentrations due to electric vehicles.

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

4. CONCLUSIONS

The authors have undertaken regional photochemical modeling 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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