Emission Inventory Preparation and Air Quality Modelling in the Pacific Northwest

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ABSTRACT

In recent years, considerable effort has been spent creating comprehensive, sub-regional emission inventories in the Pacific Northwest for use in policy reviews, planning and decision-making, and numerical modelling. Although part of an ongoing project for Environment Canada which involves a number of first-time innovations, the focus of this paper is on the steps undertaken to integrate these sub-regional data into a consistent, model-ready format. Emission processing was performed using the Sparse Matrix Operating Kernel Emission (SMOKE v1.3) modelling system and the Community Multi-scale Air Quality modelling (CMAQ) system using the RADM2 chemical mechanism. The Pacific Northwest study area covers about 700,000 km^2 and extends from central Oregon to central British Columbia, and from the Pacific Ocean west of Vancouver Island to western Idaho. Emissions, spatial surrogates, temporal factors, biogenic inputs, etc. were obtained from numerous groups and agencies, including: Environment Canada; Greater Vancouver Regional District; US EPA; States of Washington, Oregon, and Idaho; University of Washington; among others. Newly developed emission data, often varying in detail and resolution, were created, combined, and converted to SMOKE-ready format. Software tools (SMOKE-In and EI-View) developed by the authors were used to perform data compilation, processing, and QA/QC checks. Comprehensive CMAQ model evaluations for ozone and $PM_{2.5}$ show very good agreement between the modelled and observed in terms of magnitude, and temporal and spatial trends.

BACKGROUND

Poor air quality is affecting human health, and air quality remains one of the "top-of-mind" environmental concerns for Canadians (Environmental Trends: December 2001). Numerous British Columbia (BC) communities suffer from poor air quality episodes, and the British Columbia government has recently confirmed its intent to address problems in "threatened airsheds". The Georgia Basin and Puget Sound region suffers from episodes of high concentrations of air contaminants, and visibility is frequently degraded. This region is subject to increasing population growth, creating a demand for continued vigilance and action to maintain and improve air quality. Public outcry concerning the highly controversial Sumas 2 and Port Alberni power plant proposals sent a clear signal of the public's heightened concern about air pollution and associated health effects. Medical health officials in Canada and the U.S. are strongly encouraging air quality agencies to focus on ambient air quality conditions (rather than emissions estimates) as most relevant to human exposure, and at concentrations far lower than previously believed to pose a threat.

In May 2000, Environment Canada, the National Research Council, and a number of universities, and federal, provincial/state, and local agencies (the consortium) met, and agreed to a number of common standards and protocols for studying and numerically simulating air quality over the Pacific Northwest. In the intervening two years, the consortium developed and adopted a number of common factors to provide consistency amongst the consortium. For example, common domains and mapping projections were defined. Similarly, the consortium selected the Sparse Matrix Operating Kernel Emission (SMOKE v1.3) and Community Multi-scale Air Quality (CMAQ) modelling systems as the models of choice. In August 2001 the group participated in an extensive air quality data measurement field program (Pacific2001) across the Georgia Basin/Puget Sound airshed.

As part of these efforts to develop a harmonized approach, the authors have worked closely with the consortium in the past on the preparation of SMOKE model inputs for what has come to be known as the International Air Quality Modelling Project (IAQMP). The following is a list of work performed as a precursor to this project:

- Defined a 4-km resolution model grid covering the southern portions of western Canada and prepared spatial surrogates and cross-reference tables to allocate emissions to the model grid.

- Prepared temporal and speciation factors and cross-reference files.

- Developed software tools (SMOKE-In and EI-View) for formatting, editing, and visualizing emission inventory data prior to input to SMOKE.

PURPOSE AND STUDY DESIGN

Currently, a modelling initiative is underway to further improve data availability and sharing between the various groups by setting up and testing an air quality modelling environment consisting of the MC2 meteorological model, the SMOKE emission processing system and the CMAQ photochemistry transport model. The focus of the resultant project is to prepare a modelling environment that can be used to evaluate the impacts of Canadian and U.S. emissions, from man-made and natural sources, on ozone (O_3), fine particulate matter ($PM_{2.5}$) and visibility within the Pacific Northwest. This multi-phase project involves the preparation of MC2 meteorological data for input into SMOKE and CMAQ, the compilation and processing of emission inventory data through SMOKE, and performing regional air quality modelling over the entire study domain for two episodes and various trans-boundary and future year emission projection scenarios. The following is a list of tasks completed to date:

- Established an appropriate geographical extent for the modelling domain(s) and assembled the required emission inventory data and related spatial, temporal, and speciation inputs. Key data gaps in the emission inventory and related input files were identified and filled.

- Assembled 3.3-km resolution MC2 meteorological data in collaboration with Environment Canada and the University of British Columbia (UBC).

- Developed a protocol and the required software to prepare the 3.3-km resolution meteorological data for use in SMOKE and CMAQ by converting it to a suitable format and running it through the MCIP2 meteorological pre-processor.

- Defined a study period coinciding with the Pacific 2001 field study, and conducted CMAQ runs with Year 2000 Base Case emissions.

- Performed a detailed model evaluation of the CMAQ results with the Pacific 2001 field study data.

Performing this work has involved a number of first-time innovations and technical developments. The following is a list of some of the project highlights to date:

- Software was developed to convert MC2 meteorological outputs to MM5 format at 12-km and 4-km resolution;

- Software was developed to crop, re-index, and interpolate gridded surrogate data provided from various data sources to the grid spacing and model domains being used;

- SMOKE v1.3 was recompiled and run on Windows NT;

- A PC/Linux cluster running Redhat Linux v7.3 was created with: one master node (Pentium 4, 1.7 Ghz CPU, 1.0 Gb RAM, 0.5 TB RAID hard drive system, 100/200GB capacity Ultrium LTO tape drive); and, three dual-processor compute nodes (two with 2x800MHz CPUs and one with 2x750 MHz CPUs and a combined memory of 2.5 Gb RAM);

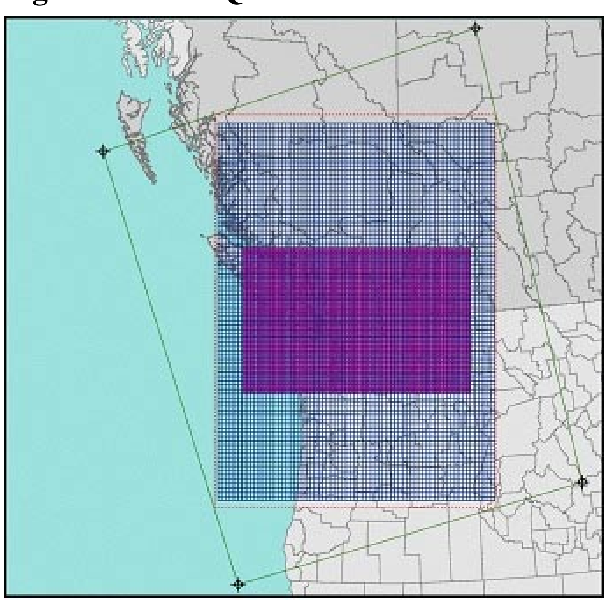
- A parallel version of CMAQ, originally compiled by the University of California at Riverside, was modified and re-compiled on the Linux cluster using the High Performance Portland Group Fortran90/C++ compiler (PGI CDK Cluster Development Kit);

- Scripts were developed to split the 12-day CMAQ runs on a day-by-day basis.

MODEL DOMAIN AND STUDY PERIOD

The aim of this project is to investigate: a) regional transport of airborne pollutants between Canada and the U.S.; and, b) air quality impacts at relatively high-resolution over the populated areas of the Lower Fraser Valley in Southern B.C. To satisfy both needs, two one-way nested domains were established as shown in Figure 1. The green outline represents the 3.3-km MC2 model domain re-projected onto the SMOKE / CMAQ Lambert Conic Conformal projection.

Figure 1. CMAQ Model Domains.



The outermost CMAQ domain is comprised of a grid with 12-km grid cells (blue grid) and extends ±500 km of the Canada / U.S. border. The inner domain (red grid) has a 4-km resolution and covers the populated areas of southern B.C. and northern Washington State.

The study period (August 9 to 20, 2001) was selected to align with the Pacific 2001 field study. The weather affecting this period was comprised of three regimes: a dry stable blocking pattern; a wet period; and finally a transient period (Snyder, 2002). The dry weather (blocking pattern) lasted until August 20, allowing pollutant levels to elevate. The synoptic patterns during the dry period can be subdivided into two phases: a stagnant phase and a well-mixed phase. Based on the discussion provided by Snyder (2002), the stagnant phase (August 10 to 15) could be described as typical of ozone episodes in this region. The well-mixed phase, however, showed ozone and PM concentrations declining as a result of increased mixing heights and the incursion of marine cloud into the region. The wet (i.e., rainy) period that followed started on August 21 and was associated with an intense low-pressure system moving south into the Gulf of Alaska. An unsettled (transient) period began after the four days of rain and persisted throughout the remainder of the Pacific 2001 experiment. The highest observed pollutant concentrations occurred during the August 10 to 15 stagnant phase.

EMISSION INVENTORY PROCESSING

For the emission inventory component, the Sparse Matrix Operator Kernel Emissions (SMOKE) modelling system was used. SMOKE version 1.3 operating on Windows NT (RWDI-version) was used to create hourly, gridded, and speciated emissions for use in CMAQ. A significant amount of pre-processing and data manipulation was required before SMOKE could be run for this study. The preparation of the emission inventory data involved the completion of the following steps:

1) *Identified data gaps in the Canadian 1995 Criteria Air Contaminant (CAC) Emission Inventory for the LFV, and fill in the gaps using the GVRD year 2000 data.* The Greater Vancouver Regional District's (GVRD's) year 2000 emission inventory for the Lower Fraser Valley (LFV) was used to fill gaps or questionable data for the GVRD and FVRD census divisions (counties) in the 1995 CAC inventory. Because the 2000 inventory contained no Source Classification Codes (SCC) for area and mobile emissions, the first task was to assign an appropriate SCC code for each emission activity type based on previous work performed by RWDI (RWDI, 2000 and 2002). This involved the creation of a comprehensive SCC Description – SCC Code mapping table using the U.S. EPA's SCC table and other resources (e.g., Environment Canada, local institutions, etc.). Temporal profile and cross reference files as well as speciation profiles files were developed and updated for all of B.C. and Alberta in SMOKE-ready format. Emissions for Whatcom County in Washington State were updated in a similar way based on updated emission data provided by the GVRD.

2) *Converted the marine emission inventory (the 2000 Canadian data and the projected 2000 US data) for GVRD into SMOKE-ready input format.* This was one of the major tasks in the preparation of the emission inventory data. The following outlines the steps taken to prepare the marine emission inventory:

- Emissions were broken out into five categories of vessels: Ocean-going, harbour, ferries, fishing and recreational vessels. Each vessel category was assigned a unique Source Classification Code (SCC) to allow for the use of unique spatial and temporal profiles.

- Five unique 'marine' counties associated with the GVRD, Vancouver Island, Whatcom County, Puget Sound, and the Washington Coast were created as shown in Figure 2.

- The five marine counties were digitized in a GIS system (ARC/INFO 8.2) based on available information from the GVRD, related and nautical charts.

- Spatial surrogates for each activity type in each county were digitized as a subset of the marine counties. Emissions from fishing and recreational vessels were allocated evenly throughout each marine county. Figures 3 to 5 show the spatial surrogates developed for Ocean-going vessels, ferries, and harbour vessels in each county, respectively.

- New temporal profiles for each vessel category were also created from information provided by the GVRD.

Figure 2. Marine Counties.

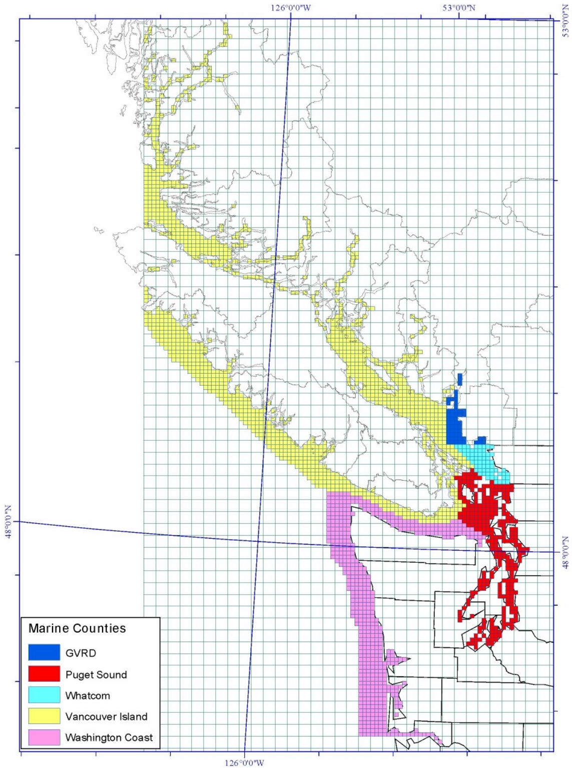


Figure 3. Spatial Surrogate for Ocean going Vessels.

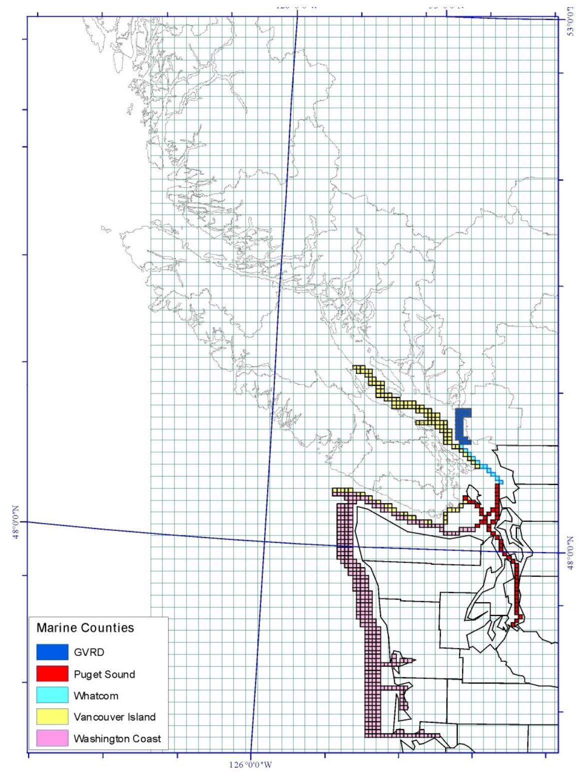


Figure 5. Spatial Surrogate for Ferries.

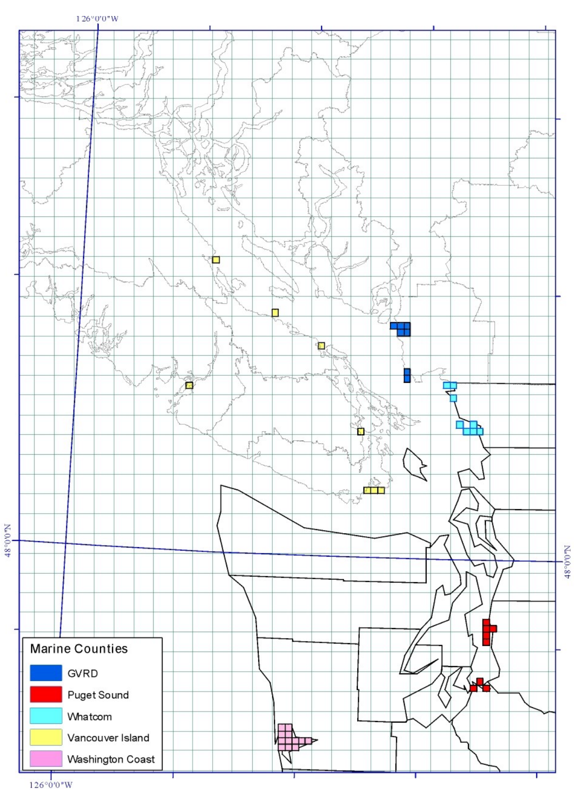
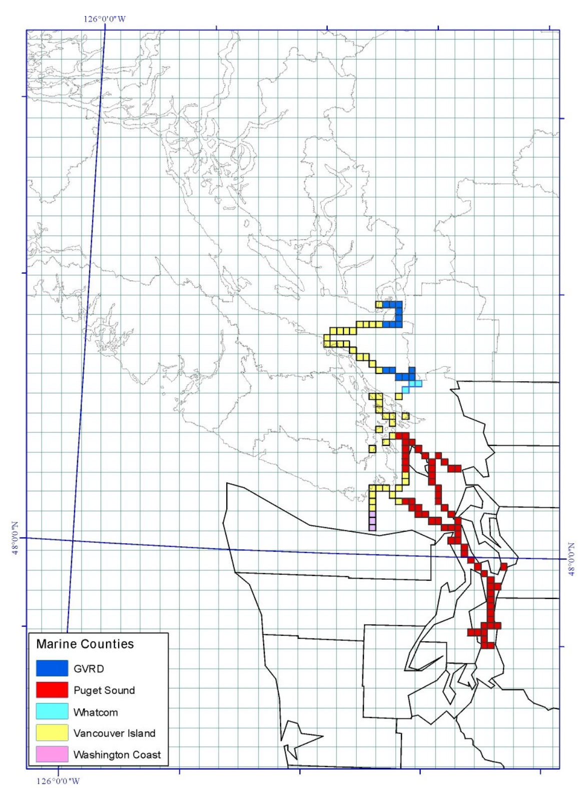


Figure 4. Spatial Surrogate for Harbours.



3) *Updated the US EPA 1996 NEI with 1999 point source data from the Washington Department of Ecology and merge the various emission files into three (one per source type) contiguous SMOKE-ready input files.* The U.S. EPA is still preparing the final version of the 1999 National Emission Inventory (NEI) data in NIF format. The Washington State DOE provided pre-released 1999 emission inventory data for point sources in spreadsheet format. However, because NH_3 emissions were missing in the 1999 EI, emissions from the 1996 EI were used instead for this pollutant.

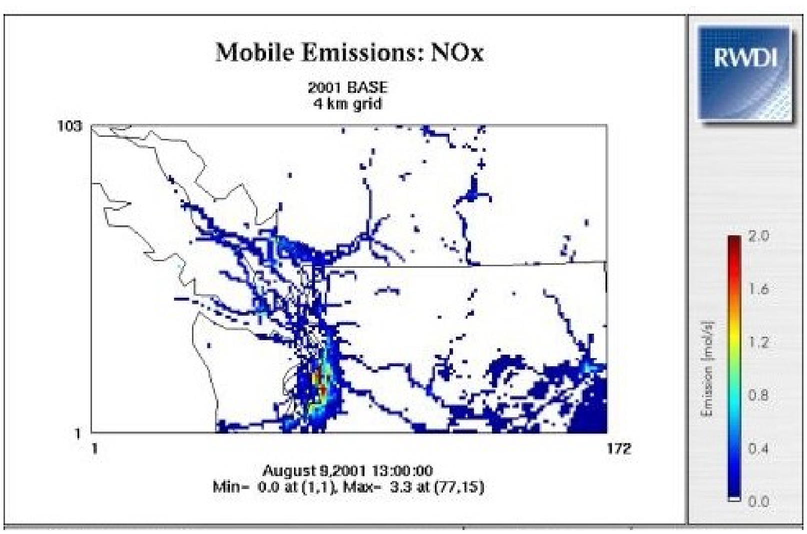
4) *Prepared Motor Vehicle Emission Data.* SMOKE was used to process both on- and off-road mobile emissions using pre-generated annual, county-wide mobile emissions data as area sources. Pre-generated 1996 on-mobile emission values grown to 2003 and provided by Washington State University were also incorporated.

5) *Prepare the Biogenic Emission Data.* Biogenic emissions refer to naturally occurring emissions of gasses from soils and vegetation. Biogenic emissions were calculated using BEIS2 based on 12-km and 4-km resolution gridded land use data and the pre-processed MC2 meteorological data. Inputs for BEIS2 were obtained from the Washington DOE for the U.S. portion of the domain, and from the data produced previously by RWDI (2002) for the Canadian portion of the domain. Emissions of NH_3 from soil (for US only) were available in the area source inventory and were modelled as area source emissions.

SMOKE RESULTS

SMOKE outputs for the August 2001 period were reviewed through the creation of summary tables and emission reports created for total emissions by pollutant (NO_X, SO_2, VOC, PM_{10}, $PM_{2.5}$, NH_3, CO) for point, area, mobile and biogenic emissions within the study domain. RWDI's SMOKE-In database tool was used to create reports from the annual emission inventory data before processing through SMOKE, allowing for the comparison of annual emission data before and after speciation, temporalization, and spatial allocation. SMOKE-In is a set of Microsoft Access databases designed to import SMOKE data from SMOKE IDA files (ASCII) and from Environment Canada's RDIS NET formatted database files. Once imported, the data can be viewed, edited, filtered, grown/projected, etc. using pre-generated queries and forms, or by using built-in database functions within MS ACCESS. Output from SMOKE-In can be generated in SMOKE-ready IDA format

Figure 6. Mobile NO_x Emissions (4-km domain)



Representative fixed-frame and animated emission plots were also examined as part of standard QA/QC practices. Both horizontal and vertical cross-sections were used to examine how SMOKE allocated the emissions in both the horizontal and vertical planes. A sample graphic representing emissions of NO_X from mobile sources only on the 4-km resolution domain at 1300 GMT (0600 LST) August 9, 2001 is shown in Figure 6. Of particular note is the replication of emissions from the marine sources and roadways both in Canada and the U.S.

CMAQ RESULTS

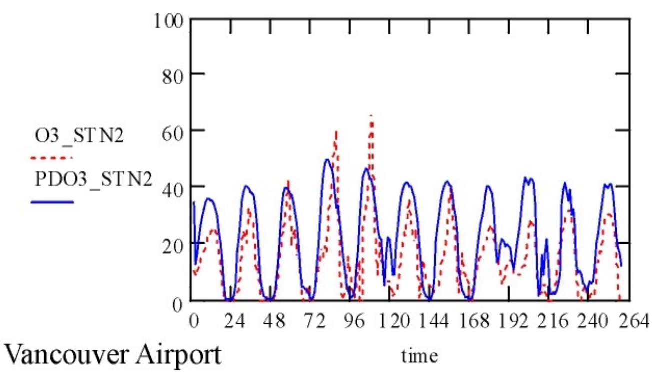
CMAQ runs were performed over the 12-km and 4-km model domains to assess its ability to replicate ozone (O_3), fine particulate matter ($PM_{2.5}$) and visibility impairment or regional haze. As noted previously, a parallel version of CMAQ was modified and installed on a PC/Linux cluster running Redhat LINUX v7.3 for this application.

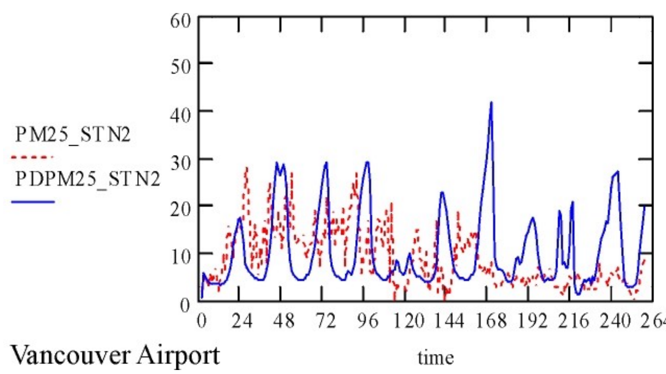
The following is a selected discussion of model performance for the 4-km resolution domain at Vancouver, an urban area where model performance was particularly good, and at Chilliwack, a predominantly rural location where CMAQ results are still good but there is evidence of some areas where difficulties were encountered within CMAQ.

Vancouver

This monitoring station was located near Vancouver International Airport and is the westernmost station used in the analysis of ozone. Predicted (PD03_STN2) and observed (O3_STN2) hourly ozone values for this station are shown in Figure 7a.

Figure 7. Modelled and Observed Ozone (a) and $PM_{2.5}$ (b) for Vancouver Airport





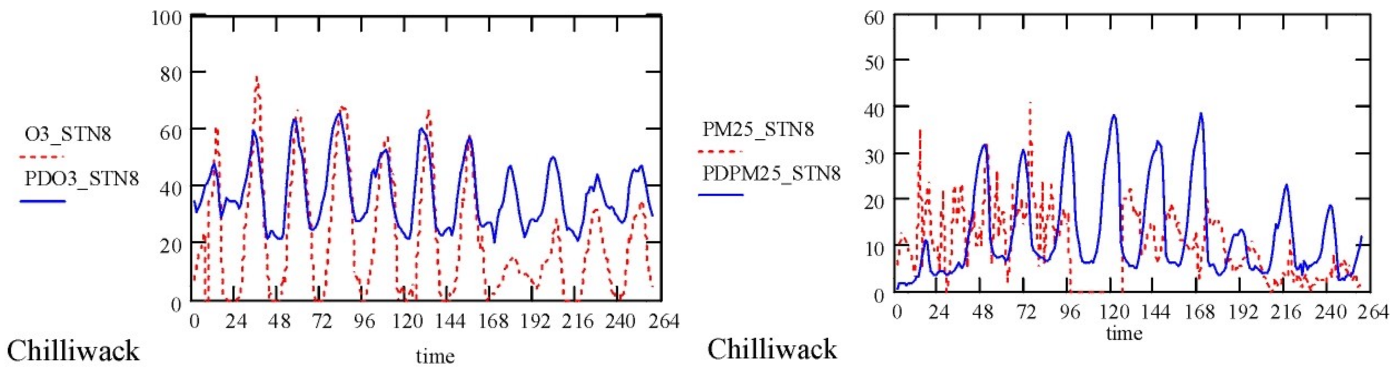
Observed ozone levels at this site were generally below 40 ppb throughout the simulation period, but climbed to about 60 ppb on days four and five of the simulation (August 13 and 14, 2001). Predicted daytime peaks were underestimated by about 15% and 30% during these two days, respectively. Overall, CMAQ performed well in terms of the replication of diurnal patterns of ozone levels. On the last four days of the simulation (August 16 through 19, i.e., the well-mixed period) and also on the first day (a spin-up day), the daytime peaks were overestimated by around 20 to 40%. On the remaining days (August 11, 12, 15 and 16) the predicted daytime peaks and night-time minimums were very close to the observed values

Modelled (PDPM25_STN2) and observed (PM25_STN2) results of $PM_{2.5}$ are shown for the Vancouver monitoring station for the 4-km domains in Figure 7b. The 4-km CMAQ results show more significant diurnal changes than was measured, especially during the dry period. The result of this is the overestimate of $PM_{2.5}$ levels at night and underestimate during the day. However, a comparison of the daily-average $PM_{2.5}$ levels indicates very good agreement between the modelled and observed. Therefore, although the model does not appear to do a particularly good job of replicating the short-term highs and lows in the $PM_{2.5}$ fluctuations, the overall prediction of $PM_{2.5}$ mass over the course of a day is quite good.

Chilliwack

The monitoring station near Chilliwack is located in the eastern half of the Lower Fraser Valley and is the farthest inland of all the stations used in the analysis. Concurrent modelled (PDO3_STN8) and observed (O3_STN8) ozone values for Chilliwack are shown in Figure 8a.

Figure 8. . Modelled and Observed Ozone (a) and $PM_{2.5}$ (b) for Chilliwack.



The model performance at this station is not as good as what is seen for the more heavily populated, western sites such as Vancouver Airport, although the model does a reasonable job of capturing the overall diurnal pattern in ozone and predicts the daytime peaks fairly closely during the stagnant phase. However, the model tends to over-predict ozone levels during the well-mixed phase. Also, the model was not successful in capturing the nighttime minimum ozone levels at this station.

The 4-km CMAQ results for $PM_{2.5}$ at Chilliwack (Figure 8b) show similar diurnal variations as those seen at Vancouver, especially during the dry period.

DISCUSSION

Overall, the MC2, SMOKE, and CMAQ modelling system performed well for predicting ozone, $PM_{2.5}$, and visibility (not shown here) at both the 12-km and 4-km resolution domains. The model does a reasonable job of capturing the overall diurnal pattern in ozone for both the 12-km and 4-km domains and predicts the daytime peaks fairly closely during the stagnant phase, although the model tends to over-predict ozone levels somewhat during the well-mixed phase. Both the 12-km and the 4-km CMAQ runs were successful in capturing the nighttime minimum ozone levels at the western, more heavily urbanized monitoring stations. Similar model performance was found for $PM_{2.5}$.

The over-prediction of ozone during the night is a common problem with photochemical model results. For this project, we believe that the primary cause may be related to the vertical structure of the model layers. Under night-time stable conditions, ozone can be significantly titrated by NO, which can result in a large vertical gradient in ozone near the surface. If the majority of the NO_X emissions are released near the surface (e.g., on-road traffic), the depth of the lowest model layer (sigma 0.995 or approximately 38 meters) is likely too high to be able to accurately capture these emissions and vertical diffusion near the ground surface. In short, the lowest level in CMAQ may not be low enough to accurately reflect the titration of ozone from low-level NO_X sources, particularly at night. In support of this argument, a review of modelled NO concentrations indicates an under-prediction at night compared to measurements at the majority of the monitoring stations. Vertical resolution may also affect the modelling of deposition processes for both ozone and $PM_{2.5}$.

There is also some evidence suggesting that eh horizontal resolution affects the prediction of ozone, especially at night (i.e., the 4-km results generally show better agreement than the 12-km results). This is likely related to the resolution of NO_X emissions, particularly in rural areas where significant local gradients in emissions can occur at scales smaller than model grid resolutions.

Overall, the diurnal patterns and magnitude of the modelled daily average $PM_{2.5}$ levels is quite good throughout the domain, with the 4-km results exhibiting better agreement than those for the 12-km domain, particularly at night. This is believed to be the result of local emission sources and the more heterogeneous nature of $PM_{2.5}$ as a pollutant compared to ozone. Secondary particulate matter can form very rapidly or slowly depending on the environmental conditions and emission source characteristics. Ozone, on the other hand, tends to form at a relatively steady rate and is therefore typically spread more homogenously throughout a given region.

The following is a summary of the factors that are expected to play a role in modelled pollutant concentrations at both the 12-km and 4-km grid resolutions.

- The representativeness of the meteorological fields provided from MC2 and converted for input to MCIP2 and eventually CMAQ can play a role in the photochemistry, as well as the mechanics of pollutant transport, dispersion, and deposition of airborne pollutants;

- The 12-km and 4-km resolutions may not be fine enough to reflect impacts associated with local emission sources, especially in the rural areas where there is a much lower density of emission sources. In urban areas, emissions tend to be more "smeared" due to the relatively high density of emission sources. In rural areas, local emissions, such as those from major roadways are spread out over 12-km or 4-km wide grid cells, resulting in increased initial diffusion / dispersion;

- The 12-km and 4-km resolutions may not be fine enough to reflect impacts associated with terrain induced sub-grid flows may affect local concentrations significantly;

- The vertical resolution used in CMAQ may play an important role in accurately predicting pollutant concentrations. For example, vertical resolution is expected to affect the resolution of nighttime inversions and deposition processes;

- The monitoring data used to evaluate model performance also have inherent limitations;

- The secondary organic aerosol chemistry modules used within CMAQ (e.g., radm2-ae2-aq) are still in a relatively early stage of development compared to those for ozone and are undergoing continuing development.

- The raw emission data are based on estimates made on a regional (i.e., county-wide) basis using a wide range of assumptions, emission factors and emission models. In addition, the disaggregation of these data to specific chemical species (in the case pf PM and VOCs), time of day, and geographic location is all based on best estimates and modelling assumptions;

CONCLUSIONS

An initiative is underway to set up and test an air quality modelling environment consisting of the MC2 meteorological model, the SMOKE emission processing system and the CMAQ photochemistry transport model to support the evaluation of impacts attributed to Canadian and U.S. emissions, from man-made and natural sources, on ozone (O_3), fine particulate matter ($PM_{2.5}$) and visibility within the Pacific Northwest. This multi-phase project involves the preparation of MC2 meteorological data for input into SMOKE and CMAQ, the compilation and processing of emission inventory data through SMOKE, and performing regional air quality modelling over the entire study domain for two episodes and various trans-boundary and future year emission projection scenarios.

To date, the initial model set up and base case modelling has been completed. Model results compare well with observed data for ozone and fine particulate matter ($PM_{2.5}$) at both 12-km and 4-km model resolutions. Additional modelling is currently underway to address the affects of a winter episode and a number of emission scenarios.

ACKNOWLEDGEMENTS

The authors wish to acknowledge a number of individuals and groups, without whom this work would not have been possible. Environment Canada (Pacific and Yukon Region) provided both technical and financial support for this project. Groups that have been involved in the preparation of model inputs include: the Greater Vancouver Regional District; University of British Columbia; the States of Washington, Oregon, and Idaho; University of Washington State; U.S. EPA Region X; and, the Pollution Data Branch of Environment Canada. The University of California at Riverside provided assistance in the recompilation of CMAQ in parallel on LINUX.

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