The SMOKE Emission Processor and Community Multi-Scale Air Quality Model (CMAQ) applied to Southern Ontario

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ABSTRACT

As part of an ongoing effort to develop regional-scale air quality modelling capabilities for photo-oxidants and atmospheric aerosols in Canada, the 1995 emission inventories for the US and eastern Canada were processed through the Sparse Matrix Operator Kernel Emissions Model (SMOKE). This was done to prepare gridded, temporalized and speciated emissions for use in the Community Multi-Scale Air Quality Model (CMAQ). SMOKE is a state-of-the-art emission inventory processing system recently developed by the MCNC Supercomputing Center in North Carolina, and CMAQ is an atmospheric chemistry/transport model developed by the US EPA and currently incorporated into their MODELS-3 modelling framework. This is the first time that the 1995 emission inventory for Canada has been processed with SMOKE. The emissions were processed to permit simulation of several scenarios so that issues of trans-boundary pollutant transport and the impact of coal-fired power plants on regional air quality in Southern Ontario could be explored. A July 1999 smog episode that produced elevated levels of ozone and $PM_{2.5}$ in Southern Ontario has been used as the test case for this study. This paper describes the many challenges that were encountered in gridding, temporalizing and speciating the Canadian emission inventory and presents some of the results of both the emission processing and the air quality modelling.

INTRODUCTION

Elevated ozone and particulate matter concentrations are a major environmental concern in heavily industrialized and populated areas throughout the world. Such concentrations often extend considerable distances downwind of the population/industry centers. In the past, Canada has set a maximum acceptable ozone concentration of 82 ppb for one hour, to protect both human and vegetative health. The region of Southern Ontario and Southern Quebec that extends from Windsor to Quebec City, the so-called Windsor Quebec corridor (WQC), exceeds this concentration level more frequently than any other part of the country (Yap et al., 1988, Reid et al. 1996). Recently, Canada established new standards for 8-hour ozone (65 ppb) and 24-hour $PM_{2.5}$ (30 $\mu g/m^3$), applicable to the 98^{th} percentile value in any three year period. These new standards are regularly exceeded in the WQC. Long-range transport is a key factor, and is affected by the interaction of large scale wind flows with lake breeze circulations over the Great Lakes (Boulton et al., 2000, Lepage et al., 2000, Hastie et al., 1999). It is important to model these effects. At the same time, it is important to reliably model the pollutant emissions at both local and regional scales, including SO_2, NO_x, VOCs and other pollutants that give rise to high

ground-level concentrations of ozone and $PM_{2.5}$ (Houyoux and Janssen, 2000, Janssen, 2000). The study discussed in this paper combined the newest emission processor, SMOKE with the CMAQ chemistry/transport model to investigate a summer smog episode in July 1999 in Southern Ontario. A base case and several emission scenarios were modelled to test the sensitivity of the CMAQ results to the emission processing.

METHODOLOGY

Overview of the Modelling System

The regional-scale air quality modelling system used in this study is comprised three main components: a meteorological model; an emission inventory processor; and a chemistry/transport model. The meteorological model used was MM5 (Version 3.0). The input to the meteorological model consisted of initial and boundary conditions derived from archived global meteorological observations at a coarse resolution. These were available from NCAR.

The emission processor used was SMOKE (Version 1), which was originally developed by the MCNC Supercomputing Center in North Carolina. SMOKE was used to produce hourly, gridded emission data from annual emission inventories provided by Environment Canada and the US Environmental Protection Agency (EPA).

The chemistry/transport model used was CMAQ (Version 2000 for the Windows™ NT platform), which was recently developed by the US EPA. This model uses the outputs from the meteorological model and the emission processor to simulate pollutant transport processes and chemical transformations in the atmosphere. CMAQ was used to predict hourly pollutant concentrations over the model grid.

Study Area

The modelling was performed first over an area or "domain" covering most of eastern North America, with a horizontal grid spacing of 36 km (**see Domain 1 in Figure 1**). Additional model simulations were performed over (a) an embedded or nested domain covering the northeastern US and southeastern Canada, with a grid spacing of 12 km, and (b) over a domain covering most of southern Ontario, northwestern New York State and northern Ohio, with a grid spacing of 4 km (**Domains 2 and 3 in Figure 1**). These runs provided improved resolution of meteorological features and emission sources in the study area. The vertical resolution of the simulation was the same for all domains. MM5 was run with 27 vertical levels, distributed between the earth's surface and 16,000 meters above ground. Fifteen of these levels were located in the lowest 3,000 meters, where the highest vertical resolution is needed. SMOKE and CMAQ were run with 15 vertical layers, ranging from the surface to 13,700 meters.

Smog Episode in July 1999

A smog episode that occurred between July 12 and July 18, 1999 was chosen as the meteorological event to be modeled. During this period, a high pressure system was centered

over the southeastern coast of the United States, resulting in clear skies and hot, southwesterly wind flows over the Great Lakes, and in particular, over southern Ontario. These are conditions that typically lead to smog events in Ontario. Temperatures in southern Ontario rose to above 30EC during the daytime. Winds were moderate, achieving mean speeds in the range of 15 to 20 km/h. **Figure 2** shows a typical pattern of surface wind and temperature fields on the 12 km domain at 2000GMT (1600EDT) on July 16, 1999.

According to the preliminary data from monitoring sites operated by the Ministry of the Environment (MOE), the peak 8-hour ozone level exceeded the new Canada-Wide Standard for ozone of 65 ppb (parts per billion). Peak hourly ozone concentrations were measured in excess of 80 ppb (Up to 100 ppb) along WQC from the Windsor, London and Kitchener areas, to Hamilton, Oakville and Toronto during this episode. The peak 24-hour $PM_{2.5}$ concentration was well above the Canada-Wide Standard of 30 $\mu g/m^3$ (micrograms of particulate matter per cubic meter of air) and hourly $PM_{2.5}$ levels rose above 60 $\mu g/m^3$.

Preparation of the Canadian Emission Inventory for SMOKE

While the 1995 emission inventory for the eastern US was mostly available in the desired format, Environment Canada's 1995 inventory for Ontario and Quebec needed to be reformatted and adapted for use in SMOKE. This involved the following steps: reformatting of Canadian point and area source emission inventory files; reformatting of Canadian mobile VMT data; reformatting of area source temporal profiles provided by Environment Canada; development of temporal profiles for Canadian point sources; merging Canadian and US inventory files and temporal profiles; merging of Canadian and US census data; development of population-based factors for distributing area source emissions to the model grids; merging US and Canadian digital road networks; development of gridded factors for distributing mobile emissions to the model grid; updating of chemical speciation profiles to include any new source types (i.e., new SCC codes) in the Canadian inventory; and updating the Canadian portion of land use data for processing biogenic emissions.

Temporal profiles for Canadian point sources were obtained using two processes: (a) using seasonal and diurnal power generation information to create unique temporal profiles for coal-fired power plants in the region, and (b) for other point sources, trying to find a reasonable match within the US temporal information that came with SMOKE. The idea was to find the closest matching US SCC to the Canadian SCC whose temporal profile we were trying to find. In cases where there was no possible match, the point source was given a default of a constant temporal profile.

While stand-alone versions of MM5, SMOKE and CMAQ were used in this study, the processing of factors (surrogate ratios) for distributing area and mobile emissions to the model grids was done using the US EPA's MODELS-3 software framework, which includes a user interface and processing software written in ArcInfo and SAS scripting languages. ArcInfo was used to merge the Canadian and US census data and road networks, making the merged data seamless at the border between the two countries. The data were then gridded to obtain the surrogate ratios, using ArcInfo and SAS routines within MODELS-3. The digital road network

for Canada used in this study was somewhat coarser than the US network, consisting only of provincial highways. For the City of Toronto, the largest city in the Canadian portion of the study area, a more detailed road network was obtained and merged with the rest of the Canadian road network. The Toronto network included all expressways and arterial roads within the city boundary.

Emissions of CO and NO_x from Canadian mobile sources were modelled using county-wide VMT data and the MOBILE5b emissions model. The MOBILE5b files and other related files that came with the SMOKE demonstration data set were used. This approach was not used for emissions of particulate matter and SO_2 from mobile sources, since the MOBILE5b files that came with SMOKE do not reflect differences in fuel sulphur content between Canada and the US. Instead, the PM and SO2 emissions were handled in the same fashion as area sources, using annual emissions and temporal profiles included in the Environment Canada emission inventory.

The Canadian point source data were lacking in stack parameters for the majority of the point sources, but the largest of the sources (coal-fired power plants and smelters) did include stack parameters. No improvements to the stack parameters were made in this study.

The use of 1995 emission data (instead of 1999 data, which were not available) in combination with a July 1999 meteorological episode resulted in added uncertainty when comparing the CMAQ model results to pollutant monitoring data for July 1999. No attempt was made to project the inventory from 1995 to 1999, except in the case of Canadian coal-fired power plants, which experienced a more significant change in emissions over that time period than any other source in the study domain. Power plant emissions increased significantly, due to a shutdown of nuclear generation facilities in Ontario. Projections from 1995 to 1999 were made based on published data from Ontario Power Generation (OPG, 2000). For some model scenarios, emissions from both Canadian and US coal-fired power plants were further adjusted to reflect anticipated NO_x reductions over the next few years.

For the processing of biogenic emissions, the biogenic land use files for SMOKE were updated with detailed land use data for Canada. These data were provided by the Ontario Ministry of the Environment.

Figure 3 shows an example of the resulting hourly, gridded emission data, as produced by SMOKE. This example is for total NO_x emissions at ground level.

MODELING RESULTS

Base Case: July 1999 Smog Event in Southern Ontario

The SMOKE and CMAQ models ran through all of the domains from 36 km, 12 km to 4 km grid-spacings. CMAQ generated hourly 3-D gridded concentrations for O_3, $PM_{2.5}$, NO_x, SO_2 and other contaminants. However, only O_3 and $PM_{2.5}$ are discussed in this paper.

<u>Ground-Level Ozone</u>

Figure 4a shows the CMAQ model results for ground-level O_3 at the 12 km grid resolution on July 16, 1999, 14:00 GMT (10:00 EDT). In the morning, a large area of high-ozone was located in eastern Michigan, west of lower Lake Huron and Lake Erie. The maximum O_3 concentration is about 80 ppb, northwest of Detroit. In Southern Ontario, O_3 levels were quite low overall at this time, except for a shallow band of ozone build-up along highway 401 from Windsor to Guelph where the predicted maximum O_3 concentration reached about 60 ppb.

The high-ozone concentration distribution pattern was much different in the afternoon. **Figure 4b** shows that a wide-spread high-ozone area moved from the US into Southern Ontario and increased its concentration up to 100 ppb. An intensive high-ozone band stretched from Windsor across London, Kitchener-Waterloo and Hamilton to the east of Toronto, indicating that mesoscale meteorological conditions in this area, such as lake breezes and lake breeze convergence zones played an important role in allocating and accumulating O_3 levels. The predicted maximum one-hour concentration for this hour was about 90 ppb to the north of Toronto. In the US, high-ozone levels appeared in southern Ohio and Pennsylvania, but not Michigan. The MM5 meteorological simulations and the meteorological observation data showed that the southwesterly wind flow consistently dominated all of the northeastern US and southern Ontario during the episode **(Figure 2)**. High temperatures and few clouds in the study area also created favourable conditions for O_3 formation. The predicted high ground-level O_3 in Ontario was mostly associated with ozone precursors (NO_x, VOCs, etc.) emitted from the upwind industrial and urban areas in the mid-western US

Ambient $PM_{2.5}$ Levels

Figures 4a and b show the predicted ground level $PM_{2.5}$ concentration at the12 km grid resolution on July 16, 1999, 14:00 GMT (10:00 EDT) and 22:00 GMT (18:00 EDT). A large, high $PM_{2.5}$ concentration area (90 ug/m^3 maximum), originally located in the mid-western United States, travelled along the southwesterly wind flow for 2-3 days moving across Michigan and Lake Huron into Ontario as shown in **Figure 5a**. Meanwhile, $PM_{2.5}$ concentrations in southern Ontario were relatively low. The afternoon $PM_{2.5}$ concentration distribution, seen in **Figure 5b,** shows a clear demarcation between the northwest and southeast parts of the 12 km domain, due to the pattern of long-range transport from the American Midwest. The maximum predicted concentration in the Toronto area was about 80 ug/m^3, but higher levels could be found in central southern Ontario. An edge of clear air indicated that a lake breeze front built up north of Lake Erie from Windsor to Hamilton. The lake breeze from Lake Erie allowed less polluted air to penetrate 10 to 20 km inland. The lake breeze effect resulted in lower $PM_{2.5}$ levels near the lakeshore than inland during the daytime.

Scenario I: Turn-off all US SO_2 Emissions, with no Change in Canadian Emissions

One of the scenarios modelled in this study was to turn off US SO_2 emissions and keep Canadian emissions unchanged. The results were then compared to the results of the base case. This scenario was implemented by zeroing out US SO_2 emissions in the SMOKE input files and then re-running SMOKE.

Change in $PM_{2.5}$ (SULF)

Sulphate aerosol was the major contributor to ambient $PM_{2.5}$ levels during this episode. Turning off the SO_2 emissions in the US had a significant affect on predicted sulphate and $PM_{2.5}$ levels in Canada. **Figure 6a** shows the base case sulphate concentrations at ground level on July 15, 1999 12:00 GMT (08:00EDT). The highest concentration (over 60 ug/m^3) was located at the southwest corner of the 12 km domain (i.e., in Indiana), while in southern Ontario the concentrations were about 20-30 ug/m^3. At this time, the sulphate concentrations in Ontario had not yet reached the peak that they would attain later on July 15 and on July 16.

Figure 6b shows the results for Scenario 1, with SO_2 emissions in the US turned off. The simulated ground level sulphate concentrations are now very low (maximum 2.3 ug/m^3) in Canada and zero in the US. Comparison with **Figure 6a** indicates that SO_2 emissions from the US were responsible for the vast majority of the predicted $PM_{2.5}$ in Canada. The contribution of Canadian SO_2 emissions to the total $PM_{2.5}$ concentration was less than 10%.

The major SO_2 emission sources responsible for the Canadian sulphate contribution shown in **Figure 6b** were power plants located south of Lake Huron and on the north shore of Lake Erie and Lake Ontario. The resulting sulphate impacts occurred hundreds of kilometers to the northeast of these sources, which is a demonstration of the fact that, during this episode, the conversion of SO_2 to sulphate occurred over very long transport distances. The long transport distances explain why US emission sources were the dominant contributors to high sulphate levels in Ontario during this event.

Change in O_3

Turning off the SO_2 emissions from the US also significantly affected O_3 concentrations in Canada. **Figure 7** shows the percentage of reduction in O_3 from the base case to Scenario 1 on July 16, 1999, 22:00 GMT (18:00 EDT). Comparing to **Figure 5b** and **Figure 4b**, the location of maximum O_3 reduction (change) in the scenario was mostly associated with the high $PM_{2.5}$ area and roughly associated with the high-ozone area in Southern Ontario. A reduction of up to 25% in O_3 concentration occurred in Southern Ontario. Evidently, the decrease in SO_2 allows an increase in the formation of nitrate aerosol. This, in turn, removes a portion of the available NO_x from the gas-phase chemistry that leads to the formation of ozone. As current smog control/reduction strategies are focused mostly on the reductions of NO_x and VOC and their effects on O_3 and particulate matter, this preliminary study leads to the additional consideration that SO_2 reduction may influence not only $PM_{2.5}$/PM_{10}, but also O_3 concentration at a significant level.

Scenario II: Reduced Emissions from a Canadian Coal-Fired Power Plant

Scenarios were run in which two new gas-turbine power plants in the Greater Toronto Area (combined capacity of 1,600 MW), displace power generation away from existing coal-fired power plants in the region. Since the existing plants have much higher emissions of NO_x and SO_2

than do gas-turbine power plants, displacing power generation away from the existing power plants would significantly reduce total emission levels without decreasing power supply. The new power plants were assumed to be equipped with Selective Catalytic Reducers (SCR's), which significantly reduce their NO_x emissions. SMOKE was used to create these emission scenarios. The results for one of these scenarios is discussed in the following paragraphs. In this scenario, the new gas-turbine power plants were assumed to be displacing power production at an existing power plant located on the north shore of Lake Erie. The resulting changes in emissions are summarized in Table 1.

Table 1: Changes in NO_x and SO_2 Emissions from Base Case to Scenario 2

Power Plant	**NO_x (tonnes/day)**	**SO_2 (tonnes/day)**
New Gas Turbines	1.7	1.0
Existing Coal-Fired	-40.5	-150.0

Change in Ozone

Figure 8 shows the predicted change in ground-level O_3 concentrations between Scenario 2 and the base case at the peak hour (12 km grid resolution). The ozone reduction area starts narrowly from the west end of Lake Ontario, extends along the north shore of the lake Ontario, impacting the cities of Toronto, Oshawa and Kingston. The width of this reduction area was predicted to vary from 10 to 50 km. The maximum reduction in concentration during the peak hour was about 2 ppb, occurring north of Toronto, which is a reduction of about 3 to 4 percent from the base case.

Change in $PM_{2.5}$

The maximum reduction in the peak 1-hour $PM_{2.5}$ concentration was only 0.5 $\mu g/m^3$ and located over Lake Ontario. It occurred on July 15, 1999, at 12:00 GMT (08:00 EDT). This was a less than a 1 percent reduction from the base case. No significant reduction in the region was predicted at any time during the 4-day model simulation. Areas of very minor $PM_{2.5}$ reduction and also some increases were found over Lake Ontario and to the northeast of the lake. The changes were predicted to occur relatively far from the sources, indicating that the formation of $PM_{2.5}$ from NO_x and SO_2 emissions occurs more slowly than the formation of O_3 which, in turn, allows for more time for dispersion of the pollutants. Overall, predicted maximum ozone reduction during the peak hour was about 4 percent, the predicted maximum SO_2 reduction was about 10 percent, and the predicted $PM_{2.5}$ reduction does not exceed 1 percent.

CONCLUSIONS

SMOKE is an efficient emission processor with little third-party software and data support required. It is relatively easy to use SMOKE to create a variety of emission scenarios under specific conditions. However, there are some limitations in the SMOKE processes such as (a) the difficulties in controlling the mobile emissions using VMT data in the input files for the Mobile 5b processor, and (b) some limited functions in the quality control and assurance tools.

By using SMOKE combined with CMAQ, we were able to study a smog episode in southern Ontario in an effective way. In the July 1999 case used for this study, the simulated high-ozone and high-PM concentrations in southern Ontario were mostly caused by the precursors emitted and transported from the Midwestern US. The SO_2 emissions, a major contributor to particulate matter, also strongly affect ground level O_3 concentrations. SMOKE/CMAQ can also be used to investigate the environmental impact from an individual major point source.

The findings of these studies are based on modeling a single, representative smog episode (July 12-17, 1999). Although the general conclusions of the studies are not expected to change for other smog episodes, the specific magnitude of predicted changes in pollutant concentrations and the locations from one episode to another are likely to change somewhat due to the very complicated nature of atmospheric chemical processes. Many important factors could affect the conclusions from one episode to another. Meteorological conditions (wind, temperature, humidity, solar radiation, precipitation, etc.), the concentrations of other chemical compounds, and the chemical mechanism used in the CMAQ model could influence the chemical reaction rate, transport, dispersion and wet/dry deposition.

Model evaluations for MM5 and CMAQ have been recently completed for the base case, using available meteorological and pollutant monitoring data for July 1999. The results show generally good agreement between the model output and observations (these results have not be presented in this paper). Further evaluations and sensitivity tests are on-going.

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