

APPLICATION OF MC2/CTM NUMERICAL MODELS AT HIGH RESOLUTION OVER SOUTHWESTERN QUEBEC AND COMPARISON WITH MEASUREMENTS FROM MAOS-MERMOZ 1996

by

Gilles Morneau Mario Benjamin Environment Canada, Quebec region

in collaboration with

Janusz Pudykiewicz Air Quality Research Branch



October 1998



3616037H

Table of contents

List of acronyms	.iii
1 Introduction	1
2 Methodology	1
2.1 The models	1
2.2 Selection of episodes	2
2.3 Meteorological situation from June 10th through 14th 1996	2
2.4 Objective analyses for the meteorological model	2
2.5 Spatial domain and grid resolution	3
2.6 Emission fields for the air quality model	3
2.7 MC2/CTM runs	4
2.8 MAOS-MERMOZ 1996 field study	4
2.9 Comparisons and tests to be performed	5
3 Results at St. Anicet and L'Assomption	7
3.1 Time series of surface ozone	7
3.2 Ozone plots	7
3.3 Time series of ozone precursors	7
3.4 Ozone at 125 and 400 metres	8
3.5 Vertical ozone profiles	8
4 Statistics of simulated vs observed data	8
4.1 Model bias and absolute error	8
4.2 Frequency distribution and 90th percentile	9
4.3 SUM60 index	9
5 Conclusion	10
6 Acknowledgements	10
References	12
Figures	13

List of acronyms

ADOM	Acid deposition and oxidant model
CEDSIO	Canadian amissions processing systems version 1.0
CEFSI.0	Canadian emissions processing systems version 1.0
CMC	Canadian Meteorological Centre
CTM	Chemical tracer model
EDT	Eastern daylight time
EMEFS-I	Eulerian model evaluation and field study for acid deposition phase I
ESOM	Etude sur les oxydants dans la région de Montréal
MAOS	Montreal area oxidants study
MC2	Mesoscale compressible community model
MERMOZ	Montreal experiment on regional mixing and ozone
NARSTO-CE	North American research strategy for tropospheric ozone - Canada east
RPN	Recherche en Prévision Numérique (Environment Canada, Dorval)
VOC	Volatile organic compound
WQC	Windsor - Quebec city (corridor)
Z	Universal time (Greenwich)

Application of MC2/CTM numerical models at high resolution over southwestern Quebec and comparison with measurements from MAOS-MERMOZ 1996

1 Introduction

Air quality models have been used for several years in Canada particularly for acid rain assessment and more recently as a tool for decision making in the troposheric ozone and smog issues. With the advent of regional smog management plans, the Quebec region must give itself tools to be able to answer the questions that will be raised. For example, what are the mecanisms responsible of tropospheric ozone formation over the Montreal area and what is the contribution of long range transport; which emission control, if any, would solve the smog problem over southern Quebec? Air quality models can contribute to resolve these questions and the purpose of this study is to apply such a model. Observations of ozone and other pollutants from the NARSTO-CE 1996 field study over southern Quebec will help validate the model and contribute to its improvement.

Specific questions adressed by this study are:

- Which horizontal scale is the best suited for regional application of these air quality models considering their current state of development?
- How useful are the models to predict surface ozone concentrations over a given area?
- How useful are the models to compute transboundary transport of ozone and its precursors?

2 Methodology

The experiment consists in using a mesoscale meteorological model to simulate the atmosphere over a short period of time during the summer of 1996, then use the results of that model as input to an air quality model to obtain concentrations of ozone and its precursors. In order to reproduce the most accurately as possible the atmospheric conditions that prevailed during the selected period, the meteorological model is nested inside objective analyses of meteorological fields throughout the integration. Objective analyses are produced by the Canadian Meteorological Centre (CMC) as a part of their global and regional data assimilation process and are the best available estimations of the true meteorological fields. The mesoscale meteorological model then becomes an interpolator in time and space of these objective analyses and a generator of fields that are not available in them such as most boundary layer and precipitation variables.

2.1 The models

The air quality model used is the Chemical Tracer Model (Pudykiewicz *et al.*, 1997) henceforth called CTM. The CTM model incorporates accurate semi-Lagrangian advection

and ADOM II comprehensive chemistry including 114 reactions between 47 chemical species (Lurmann, Lloyd and Atkinson, 1986; MacDonald *et al.*, 1993). The meteorological variables needed by CTM during its integration, such as winds, air temperatures and stability, will be provided by the Mesoscale Compressible Community model MC2 (Tanguay *et al.*, 1990; Benoit *et al.*, 1997). The meteorological model MC2 is based on a fully compressible set of primitive equations solved using a semi-implicit and semi-Lagrangian method. The physical parameterization used in MC2 is the one currently in operation at the Canadian Meteorological Centre. The combination of MC2 with CTM has been widely used for the Canadian 1996 NOx/VOC science assessment where they were compared to other models and observations¹.

2.2 Selection of episodes

We intend to assess the air quality model over a time period for which the surface ozone concentrations reached values near or above the canadian objective of 82 parts per billion. During MAOS-MERMOZ 1996 field study, such concentrations were reported over southern Quebec on the 11th and 12th of June and on four consecutive days east of Montreal from August 4th through August 7th. Unfortunately, a single period could be simulated in the context of this study due to limited computer resources. The selected period is the June episode, the primary reason for this choice being the availability of more field measurements from June 10th to 14th than during the August episode. However, we intend to simulate the August episode in future work.

In order to study the period of June 10th to 14th 1996, both the meteorological and chemistry models will be run from June 7th, mainly to get a longer period of time to do the assessment and to ensure that long range transport influences are fully taken into account by the 10th.

2.3 Meteorological situation from June 10th through 14th 1996

Meteorological situation during this period was characterized by a high pressure system over the Atlantic ocean and various low pressure systems over centre and northern part of the continent, resulting in a weak south to southwesterly flow over southern Quebec up to the 14th. The winds then shifted to the west after the passing of a trough during the day. The weather on June 10th over southern Quebec was mostly cloudy with showers and light northeast to southeasterly winds. On the 11th and 12th, it was mostly sunny with a few showers during the night and light southerly winds. On the 13th, cloudy skies with showers and thundershowers and light south to southwesterly winds were observed. The 14th was mostly cloudy with scattered showers then clearing in the afternoon with winds shifting to the west and increasing to moderate.

2.4 Objective analyses for the meteorological model

Objective analyses of meteorological fields were retrieved from CMC archives for the period of June 7 to June 15 1996. The regional analyses are available every 6 hours at a resolution of 35 km over North America. The analyses are composed of 2-dimensional fields (surface pressure, soil humidity, surface and deep soil temperatures, snow depth and cover, albedo, ice cover) and of 3-dimensional fields divided into 28 vertical sigma levels (virtual

¹ Modelling of ground-level ozone in the Windsor-Québec City Corridor and in the Southern Atlantic Region. Report of the WQC Corridor and Southern Atlantic Region modelling and measurement working group. Environment Canada, 1997, 265 p.

temperature, specific humidity and horizontal winds). Geophysical fields needed by the model, such as vegetation type, land-sea mask, roughness length and topography variance, were obtained from climatological files and maintained constants throughout the simulation period. The objective analyses provide initial values for MC2 variables and the lateral boundary conditions during the integration of the model.

2.5 Spatial domain and grid resolution

The spatial extent of the simulations has to be determined. The purpose of the experiment is to study tropospheric ozone and its precursors over southern Quebec. The local oxidant chemistry is influenced by long range transport and this fact must be taken into account. The ideal domain would therefore encompass all sources of pollutants that could affect oxidant chemistry over southern Ouebec. Since the lifetime of some ozone precursors is as long as a few days, such a domain would have to cover most of North America. Unfortunately, limited computer resources impose some compromise. We have to choose a domain wide enough to cover the main source regions while at the same time being not too big as to exceed hardware capacity. The most limiting factor as far as hardware is concerned is the CTM grid size which cannot exceed 70 by 70 points horizontally with 20 vertical levels. This consideration suggests that the MC2 grid could be defined as 100 by 100 points horizontally with 29 vertical levels. The MC2 grid is larger than the CTM grid to allow extra space on each side for a sponge zone required to set the lateral boundary conditions. The proposed configuration leaves enough space for a transition zone of 15 points wide even though the actual value that was used in the experiment is 10 points. The number of vertical levels in MC2 is set to 29, a commonly used value when integrating the model for mesoscale studies.

To determine which horizontal scale is best adapted for regional applications, both models will be run at two different resolutions. Resolution in this context is to be interpreted as distance between adjacent grid point in the model grid. Since the objective analyses have a resolution of 35 km and that current model parameterizations impose a lower limit of about 12 km, it was decided that MC2 and CTM would be run on a 35 km resolution grid, then run on a 12 km resolution grid. The former grid is called the coarse grid and the latter is called the fine grid. Note that the model grids are set on a polar stereographic projection true at 60° N, therefore the specified resolutions are also true at 60° N. The whole domain covered by our MC2 grid of 80 by 80 points, once the sponge zone has been removed, is shown on figure 2.1 for the two resolutions. The center of both grids were slightly offset to the southwest of the area of interest to include most long range transport effects since the prevailing direction of low level winds is southwest. One can notice from figure 2.1 that the fine grid covers a much smaller area than the coarse grid since the number of grid points is constant. The high resolution domain lacks many important source regions such as the Midwest and the industrialized east south of New York. In this case, we are sacrificing long range transport for better resolution. Concentrations of chemical species obtained from CTM on the coarse grid could however be used to set the lateral boundary conditions for the smaller domain, higher resolution simulation. This would allow transport of pollutants into the fine grid domain from the outside world. Such an experiment is planned to be done in the future.

2.6 Emission fields for the air quality model

The life cycle of an atmospheric pollutant is composed of its emission into the atmosphere, its transport and diffusion by the atmospheric flow, chemical or photochemical

transformations with other species and finally its scavenging to the earth surface. The CTM model, with the help of the meteorological model, handles most of these processes except the emissions into the atmosphere. This data is provided in a separate database which must be updated regularly to reflect changes in pollutant sources. Ideally, the data should also be available at the finest resolution needed by the model. The emission fields that are used in this experiment are the ones used for the 1996 NOx/VOC assessment report and are based on 1985 emission inventories. The emission data is best described in appendix 3B of the assessment report². The biogenic emissions in this dataset are valid for the period of EMEFS-I field study of August 1988, not for the period of June 7 to 14 1996 for which it is used. When the Canadian Emission Processor System CEPS1 becomes available, we will be able to incorporate more recent emission inventories and get more realistic values for temperature-dependent data such as the biogenic emissions.

2.7 MC2/CTM runs

MC2/CTM wil be used to simulate the period of June 7th to June 14th 1996. The MC2 meteorological model will be integrated one day at a time with fresh initial conditions. The integration is started at 1800Z the previous day and is carried out for 30 hours. The first 6 hours of integration allow the model to reach internal balance and are discarded, leaving 24 hours of meteorological fields to drive the air quality model. On the coarse grid, the nesting fields for MC2 will be the objective analyses provided by CMC, whereas on the fine grid the nesting fields will be the MC2 outputs obtained from the coarse grid integrations (this process is called a cascade). The output fields of MC2 are saved every hour to accomodate the needs of CTM. The MC2 time step is set to 450 seconds for the integration on the coarse grid and brought down to 150 seconds on the fine grid.

The air quality model is run on a 70 by 70 sub-grid of the MC2 model at both resolutions. The CTM grid is obtained from MC2's free domain of 80 by 80 points by removing a border of 5 grid points from each of the four sides. The time step of CTM is one hour on both grids and is run 24 hours at a time. The concentrations at the lateral boundaries of the model grid are not treated in any particular fashion during the integration (whether set to a background value or, for the fine grid, taken from the coarser 35 km grid). This is a weakness that will be treated in future work, most specifically for the inner fine grid.

2.8 MAOS-MERMOZ 1996 field study

Several measurements of pollutants, such as O_3 , NO_x , CO, VOC, are available over southern Quebec during the summer 1996 MAOS-MERMOZ field study. Figure 2.2 shows the air quality station network comprising several rural and urban sites providing surface measurements along with two upper air sites (St. Anicet and L'Assomption). Species measured at surface stations include O_3 , NO_2 , NO, SO_2 , CO. At St. Anicet and L'Assomption, additional VOC species are measured along with full surface meteorology. These two stations also provide ozone concentrations aloft measured with tethersondes, and vertical profiles of winds, temperatures and humidity. Surface observations are available on an hourly basis whereas upper air soundings are available at a few hours in the morning and

² Modelling of ground-level ozone in the Windsor-Quebec City Corridor and in the Southern Atlantic Region. Report of the WQC Corridor and Southern Atlantic Region modelling and measurement working group. Environment Canada, 1997, 265 p.

in the late afternoon. Table 2.1 lists the stations for which the measurements were compared to model outputs in this particular study.

2.9 Comparisons and tests to be performed

This study will verify how the CTM model reproduces the atmospheric chemistry of ozone over southern Quebec and if the use of a higher resolution improves the results at the cost of more computer resources. We will compare observations, at the surface and aloft, with outputs of CTM at both resolutions of 12 and 35 km. We will not assess the meteorological driver MC2 in this particular study. A short assessment of the MC2 model for the selected episode is available in the MERMOZ project report³.

The first results shown in the next section are time series of surface ozone for both St. Anicet and L'Assomption stations, followed by ozone concentrations at 125 and 400 metres above the ground at L'Assomption. We will also compare the time series of the concentrations of some ozone precursors at L'Assomption, namely NO_x and some VOC's.

The second results shown will be O_3 soundings taken at L'Assomption (tethersondes) between June 10th and June 14th. They will be compared with the vertical profile of ozone simulated by the model.

The remaining tests deal with surface ozone concentrations measured by the entire network. Our goal is to compare both measured and modelled ozone upwind, downwind and in the urban region of Montreal. Thus the whole region is divided into three subregions (see table 2.1):

- 1- northeast region of Montreal (denoted NE in table 2.1) including all rural sites of the northeast and one suburban site (Varennes), for a total of 7 stations;
- 2- the southwest of Montreal (denoted SW) including the rural sites of the southwest plus one suburban site (Dorval), for a total of 3 stations;
- 3- the urban region of Montreal (denoted MTL) comprising the remaining 10 stations.

We will compute the mean model bias and absolute error for all hours for each subregion, and again for all hours during daytime (between 7:00 AM and 8:00 PM). We will also compute the model bias and absolute error in predicting the daily maximum ozone concentration for each subregion. The frequency of hourly concentrations will then be plotted and the model compared to the observations. As a last test, we will compare the SUM60 index, a summation of all hourly concentrations above 60 ppb, for each station. Although this index is normally used to assess the effect of high ozone concentrations on vegetation during the growing season, it will give us an estimate of the model bias and error for the selected episode.

³ MERMOZ Project Report. Recherche en Prévision Numérique, Environment Canada, 1997.

Table 2.1

,

This table shows the location of each measurement station, its type and the subregion it belongs to. The type is R for rural, SU for suburban and U for urban. Longitudes west of Greenwich are negative. Three subregions are defined, namely NE, northeast of Montreal, SW, southwest of Montreal, and MTL which includes all urban sites of the metropolitan area.

Code	Station name	Туре	Latitude	Longitude	Subregion
WHM	Varennes	SU	45.717	-73.383	NE
WEW	L'Assomption	R	45.817	-73.433	NE
WBZ	Saint-Anicet	R	45.117	-74.283	SW
WVY	Sainte-Francoise	R	46.450	-71.917	NE
LON	Longueuil (Cure Poirier)	U	45.514	-73.486	MTL
BRO	Brossard(Parc Oc.)	SU	45.439	-73.469	MTL
LAV	Laval (Arena Chomedey)	U	45.547	-73.747	MTL
REM	Saint-Remi	R	45.205	-73.644	SW
CHR	Charette	R	46.436	-72.886	NE
ZEP	Saint-Zephirin	R	46.042	-72.660	NE
TIN	Tingwick	R	45.901	-71.939	NE
SIM	Saint-Simon	R	45.709	-72.835	NE
BOT	Jardin Botanique	U	45.557	-73.574	MTL
ONT	Rue Ontario	U	45.522	-73.558	MTL
AUT	Decarie-Duncan	U	45.502	-73.656	MTL
MTN	Montreal-Nord (Parc Pilon)	U	45.587	-73.636	MTL
PEL	Peel-Maisonneuve	U	45.501	-73.575	MTL
VER	Verdun (St. Joseph)	U	45.472	-73.575	MTL
ROX	Roxboro (4th Ave)	U	45.487	-73.805	MTL
DOR	Dorval	SU	45.434	-73.729	SW

Application of MC2/CTM at high resolution

3 Results at St. Anicet and L'Assomption

3.1 Time series of surface ozone

Figures 3.1a and 3.1b show the observed surface ozone concentrations at L'Assomption and St. Anicet compared with CTM outputs for both 35 and 12 km grids. The model values for a station location are obtained by linear interpolation of the values at the model grid points. In figure 3.1a, we see that CTM did quite well at simulating surface ozone concentrations at L'Assomption, specially on the afternoons of the 11th and 12th. However, the CTM peak on the 10th did not materialize in the observations. Let's recall that on this particular day the weather was cloudy and foggy with showers and that the model doesn't handle wet scavenging nor does it contain liquid phase chemistry. In figure 3.1b, the 35 and 12 km model solutions differ quite sensibly for St. Anicet and it appears that the observations lie in between the two model solutions in the afternoons. However, during night hours, the model on the 12 km grid brings ozone concentrations closer to the observations.

3.2 Ozone plots

The spatial distribution of simulated surface ozone concentrations and winds at 3:00 PM EDT (1900Z) on June 10th is plotted on figure 3.2a. The predicted maximum of 80 to 90 ppb in the L'Assomption region is clearly visible but was not observed, possibly due to the fact that the weather was cloudy with showers all day.

Figures 3.2b and 3.2c illustrate the daily maximum ozone concentrations for June 11th and 12th predicted by the model. On these days, the maximum observed in the L'Assomption area northeast of Montreal were well simulated by the model.

Figures 3.2a and 3.2c highlight a transport of pollutants from the New York and Philadelphia regions along the Hudson and Richelieu river valleys under southerly winds conditions. The model shows that this source of pollutants, combined with the contribution of Montreal, gives high ozone concentrations in the L'Assomption region when winds are from the south. The analysis of observations at L'Assomption during MAOS-MERMOZ 1996 supports this fact. The maximum ozone concentrations at the surface occur under south-southeasterly winds conditions (Robichaud and Benjamin, 1998).

3.3 Time series of ozone precursors

The time series of NO, NO_2 and NO_x are plotted on figures 3.3 for L'Assomption. The solution on the fine grid shows better agreement between the model and observations when the concentrations are low. However, the early morning peaks on the 11, 12 and 13th seem to be handled better on the 35 km grid.

Figures 3.4a to 3.4f show the concentrations of some volatile organic compounds measured at L'Assomption along with equivalent CTM outputs on both the coarse and fine grids. The simulated values agree most of the time with the observations except for methyl-ethyl-ketone (MEK) which is always overestimated by the model. High observed concentrations of propane, toluene and isoprene on June 11th were not predicted by the model. The situation concerning these pollutants was very specific on this day: the values of observed concentrations were abnormally high on the 11th of June compared to the rest of the season

(A. Robichaud, personal communication). Data analysis of summer observations at L'Assomption (Robichaud and Benjamin, 1998) reveals that concentrations of propane and toluene were on that day about 10 times higher than the summer average, whereas the concentrations of isoprene were 3 times higher.

3.4 Ozone at 125 and 400 metres

Figures 3.5a and 3.5b show the ozone concentrations at 125 m and 400 m above ground as a function of time for L'Assomption. The model values at these levels at L'Assomption were obtained by linear interpolation in the same fashion as for surface data. In figure 3.5a, one can notice that the modeled concentrations of ozone at 125 m are always too high in the morning. We will examine this fact more thoroughly in the next paragraph (3.5). However, in the afternoons, the fine grid solution is close to observations. At 400 m, figure 3.5b shows that the 12 km model agrees better with the observations but values are again overestimated in the morning of the 10th and 11th. On the 13th, the model shows a clear diurnal variation at 400 m whereas the observations don't show such a diurnal trend.

3.5 Vertical ozone profiles

The vertical profiles of ozone concentrations at L'Assomption were retrieved from the MAOS soundings for which data is available up to 400 metres above ground. A few soundings were done in the morning and a few more in the afternoon between June 10 and June 14. Figure 3.6 depicts nine such soundings compared to the model vertical profile of ozone on the 12 km and 35 km grids. In general the modeled concentrations are too high, although the 12 km grid solution is closer to the observations. It would be interesting to see if the model also overestimates ozone concentrations aloft upwind of Montreal at St. Anicet. Unfortunately, no ozone sounding was done at St. Anicet during this period. We expect such an experiment to be done in the future in order to help us evaluate the liability of the model to compute transport and fluxes of ozone and its precursors.

Figure 3.6 also tells us that the surface layer where concentrations remain low (e.g. below 20 ppb) until late in the morning is too shallow in the model. On June 12th, 1100Z and June 13th, 1000Z, the observed thickness of this surface layer is about 150 m while it is at most 50 to 60 m in the model. Furthermore, after 1200Z, this layer disappears in the model but continues to be present in the observations. This weakness of the model might be due to the treatment of the boundary layer in the meteorological driver and should be investigated further.

4 Statistics of simulated vs observed data

We will compare in this section model outputs to observed values of ozone concentrations available from the surface network. The predicted hourly ozone concentrations on both grids was linearly interpolated to each station listed in table 2.1. The comparisons are made either for all stations taken as a whole, either separated in three subregions.

4.1 Model bias and absolute error

Figure 4.1 depicts the mean model bias (predicted value minus observed value) and the mean absolute error at both resolutions using all hourly values of ozone concentrations.

Comparison is done also using only daytime values from 7:00 AM to 8:00 PM in order to test the model's ability to reproduce photochemical ozone production. From this figure, we see that the 12 km grid simulation has the smallest bias and absolute error for all regions, whether for the whole day or for daytime values only. Mean bias is positive and goes from 3 to 7 ppb and mean absolute error from 12 to 15 ppb. Bias and errors are somewhat greater for daytime than for the whole day which indicates that the model perhaps overestimates the daytime production of ozone.

Figure 4.2 compares the daily maximum values on a subregion basis. Both rural regions, upwind and downwind of Montreal, are compared separately and then taken as one. This test is unpaired in space and time. For a given subregion on a given day, the maximum value of ozone concentrations predicted by the model for any station on any hour is compared to the observed maximum in the subregion, without requiring the station or hour to be the same. The model on the fine grid has the best results for all subregions with an error of 14 ppb and a positive bias of 11 ppb. The model bias and error on the fine grid show little variation from one subregion to another, unlike the solution on the coarse grid where the errors for the southwest subregion is clearly greater than for the northeast subregion.

4.2 Frequency distribution and 90th percentile

The frequency distribution of ozone concentrations is plotted on figure 4.3. The upper graph shows data for the 10 rural stations and the lower graph data for all 20 stations together. An analysis of the figures indicates that for the period under study the model doesn't predict enough low concentrations (below 20 ppb) and predicts too often high concentrations (above 60 ppb). The model solutions on the two grids are generally close together in the mid-range (20-60 ppb) but the 12 km grid values are closer to the observations in the low and high ends of the distribution.

The analysis of percentile values is a complement to the analysis of the frequency distribution. The 90th percentile indicates the concentration level below which 90 percent of the observed or simulated values will lie. Figure 4.4 shows the 90th percentile ozone concentration for modelled and observed ozone values for each subregion. In the rural subregions, one can see that10 percent of the observations are above 48 ppb whereas the model has a value 52-56 ppb on the fine grid and near 70 ppb on the coarse grid. That is to say, the model overpredicts the high concentrations, but that the 12 km grid gives smaller differences than the 35 km grid.

4.3 SUM60 index

The SUM60 index was developped for vegetation damage caused by concentrations of ozone exceeding 60 ppb, but is also used as a general indicator of potential effects due to high concentrations. SUM60 is defined as the sum of all hourly concentrations above 60 ppb in the selected interval of time. In our case, the summation has been calculated for a period of 7 days, from June 8th 0000Z to June 14th 2400Z. Figure 4.5 is a plot of the mean model bias and absolute error when simulating the SUM60 index. As expected from previous results, the bias is positive. The graph shows that CTM on the fine grid produces an index having an error about 8 times lesser than CTM on the coarse grid does.

5 Conclusion

We have shown in this study that the CTM model was able to reproduce the main features of ozone concentrations and of nitrogen oxides precursors quite fairly during the selected episode. The model outputs were compared with measurements from the MAOS-MERMOZ field study of the summer 1996. Observations of surface ozone from 20 stations were used to compute the statistics. Concentrations of ozone precursors and vertical ozone profile available at L'Assomption were also analysed.

For the period of June 8th to 14th 1996, the model generally overestimates surface ozone concentrations over southern Quebec, whether on the coarse or on the fine grid. The model also overestimates ozone concentrations at all levels up to 400 metres at L'Assomption. The model solution on the fine grid gives the smaller errors for the surface data, its mean bias being about 3 times lesser and its mean absolute error being 25 percent smaller than the solution on the coarse grid. The mean bias and error are much more constant in space at the 12 km resolution, the values for upwind and downwind regions being almost equal.

Upper air observations of ozone at L'Assomption reveal that the surface layer characterized by low ozone concentrations at night and in the morning breaks down too early in the model. This problem could be due to the treatment of the boundary layer in MC2, but this has to be examined further.

Frequency distribution graphs indicate that ozone concentrations above 40 ppb occur too often in the model, but the solution on the 12 km grid is clearly closer to the observations.

Questions and improvements to be adressed are:

1- Incorporation of true long range transport of chemicals in the smaller 12 km resolution grid;

2- Use of more recent, better quality emission inventories;

3- Integrate the model for longer time periods to cover a greater range of meteorological conditions;

4- More thorough assessment of vertical profiles of ozone concentrations and other meteorological variables in the model using observations at St. Anicet and L'Assomption.

In light of the above results, recommendations are to definitely pursue the use of the model at high resolution for regional issues, and that other simulations and comparisons be done using other and longer time periods.

6 Acknowledgements

The authors of this study would like to thank the NOx/VOC science program for the financial funding. Special thanks to S. Venkatesh for providing us the needed ressources to run MC2 on the supercomputer and to Jocelyn Mailhot, Robert Benoit and Michel Desgagné of RPN for their support and training to use MC2. Data from the Montreal Urban Community stations were provided by Claude Gagnon and those from the Quebec ministry of Environment and Wildlife (Ministère de l'Environment et de la Faune du Québec) stations by Richard Leduc. Tom Dann of Environment Canada provided VOC and aldehydes analyses at L'Assomption. Thanks to Alain Robichaud for providing us with useful information and computations of the SUM60 index. The authors would also like to

thank Marc Beauchemin for the revision of the text and the useful comments that was provided.

References

- Benoit, R., M. Desgagné, P. Pellerin, S. Pellerin, Y. Chartier and S. Desjardins, 1997: The Canadian MC2: A Semi-Lagrangian, Semi-Implicit Wideband Atmospheric Model Suited for Finescale Process Studies and Simulation. *Monthly Weather Review*, **125**, 2382-2415.
- Lurmann, F. W., A. C. Lloyd and R. Atkinson, 1986: A Chemical Mecanism for Use in Long-Range Transport/Acid Deposition Computer Modeling. *Journal of Geophysical Research*, 91, D10, 10905-10936.
- MacDonald, A. M., C. M. Banic, W. R. Leaitch and K. J. Puckett, 1993: Evaluation of the Eulerian Acid Deposition and Oxidant Model (ADOM) with Summer 1988 Aircraft Data. Atmospheric Environment, 27A, 1019-1034.
- Pudykiewicz, J. A., A. Kallaur and P. K. Smolarkiewicz, 1997: Semi-Lagrangian modelling of tropospheric ozone. *Tellus*, **49B**, 231-248.
- Robichaud, Alain and Mario Benjamin, 1998: Analyse statistique multivariée des données de surface à la station de L'Assomption (ESOM-96). Internal report, Atmospheric Environment Branch, Quebec region, Environment Canada, May 1998. (Available from Mario Benjamin, Environment Canada, 100 Alexis-Nihon blvd, suite 300, Saint-Laurent, Canada H4M 2N8; e-mail: mario.benjamin@ec.gc.ca)
- Tanguay, M., A. Robert and R. Laprise, 1990: A semi-implicit semi-Lagrangian fully compressible regional forecast model. *Monthly Weather Review*, **118**, 1970-1980.



Figure 2.1 The top figure shows the free domain of 80 by 80 points inside the MC2 integration grids. A: the coarse grid at a resolution of 35 km; B: the fine grid at a resolution of 12 km. The bottom figures depict the grid mesh over southern Quebec at both resolutions.











Figure 3.2a Model output for June 10th at 3:00 PM EDT (1900Z) showing ozone concentrations and surface winds. The top figure is the solution on the 12 km grid and the bottom figure in on the 35 km grid. Units of ozone concentrations on the figures are 10 ppb.





Figure 3.2b Daily maximum concentration of ozone predicted by the model on the 12 km grid (top) and the 35 km grid (bottom) on June 1 lth 1996. The units of ozone concentrations on the scale are 10 ppb. Afternoon (3:00 PM) winds from the model at the 300 metres level are also plotted on the upper figure.





Figure 3.2c Daily maximum concentration of ozone predicted by the model on the 12 km grid (top) and the 35 km grid (bottom) on June 12th 1996. The units of ozone concentrations on the scale are 10 ppb. Afternoon (3:00 PM) winds from the model at the 300 metres level are also plotted on the upper figure.



Figure 3.3 Time series of nitrogen oxides concentrations at L'Assomption, (a) NO_2 , (b) NO and (c) NO_x (on next page).



Figure 3.3c Time series of NO_x concentrations at L'Assomption.



 Figure 3.4 values.
 Comparison between measurements of selected VOC's at L'Assomption and the model

 21





Figure 3.5 Time series of ozone concentrations at L'Assomption (a) 125 metres above ground and (b) 400 metres above ground.



Figure 3.6 Vertical profile of ozone concentrations at L'Assomption obtained from tethersondes during the morning and afternoon between June 10th and June 14th 1996.



Figure 4.1 Mean model error for each region for all hours (except from 7 AM to 8 PM where daytime is specified). The rural region includes the southwest subregion plus the northeast subregion. The top figure shows the model mean bias and the bottom figure shows the mean absolute error.



Figure 4.2 Mean model error in predicting the daily maximum ozone concentration for the two rural regions. This test is unpaired in space and time, that is, for a particular day and region, the maximum concentration predicted by the model at any station and hour is compared with the maximum observed in the region for that day. The top figure shows the model mean bias and the bottom figure shows the mean absolute error.





Figure 4.3 Frequency distribution of ozone concentrations for the hourly observed and simulated values. Top: non-urban stations only (10 stations, regions SW and NE). Bottom: all 20 stations.



Figure 4.4 90th percentile ozone concentration for the hourly observed and simulated values. The 90th percentile is the concentration value below which 90 percent of the hourly ozone concentrations are observed or predicted.



Figure 4.5 Mean model bias and absolute error for the SUM60 indices. The averages were computed using the 10 rural stations only then using all the 20 available stations. The SUM60 summations were performed over a period of 7 days from June 8th to June 14th 1996.