

Progress report to the Canadian Institute for Research in Atmospheric Chemistry on
**OXIDATION CHEMISTRY IN
SOUTHERN ONTARIO:
THE SONTOS '96 STUDY**

D. R. HASTIE^{1,2}, J. C. McCONNELL^{2,3}
J. NARAYAN^{1,2}, D. PLUMMER^{2,3},
J. W. DRUMMOND², V. YOUNG^{1,2},
J. KAMINSKI^{2,3}, L. NEARY^{2,3}, and M. SADEK^{2,3}

D. R. HASTIE, and J. C. McCONNELL
Principal Investigators

¹Department of Chemistry
²Centre for Atmospheric Chemistry
³Department of Earth and Atmospheric Science
York University
4700 Keele St.
North York, Ontario M3J 1P3.

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ABSTRACT

This report outlines the progress up to the end of June 1997 on the CIRAC project AOxidation Chemistry in Southern Ontario@. This encompasses the data related activities of the York University group following on the January 24 1997 report, and the first results of the modelling activity.

As part of the SONTOS program, measurements related both to smog formation and emissions inventories were made at the Binbrook site and from a light aircraft. This preliminary report deals primarily with the data obtained from the aircraft and its use in conjunction with a photochemical model in order to assess the emission inventory for the Greater Toronto Area (GTA). Measurements of temperature, O₃, NO_x, and hydrocarbons were obtained from 5 of the 6 flights undertaken. The data are presented in the Appendix. In order to assess the GTA emissions, we have chosen meteorological conditions such that the flow was from the North West. In this the analysis is less confused with emissions from other sources transported in the region. We have started with the data from Saturday August 24 1996. On this day there was steady North Westerly

flow, and measurements were made upwind and downwind of the city. The upwind measurements have been used to set initial conditions for a 3-D Eulerian model, the model is the state of the science, MC2 meteorological model with embedded emission, dry deposition, chemical reaction, and photolysis rate modules, run at a resolution of 5.3 km². The outputs from the model are compared with the downwind measurements from the aircraft.

The results are preliminary and only a single day has been simulated, but it appears as if the model, with its embedded emission module, underestimates both NO_x and VOC concentrations immediately downwind of the city. Additional computer model runs are being performed to estimate an emission data set which is consistent with the measurements.

INTRODUCTION

This report outlines the progress up to the end of June 1997 on the CIRAC project AOxidation Chemistry in Southern Ontario@. This encompasses the data related activities of the York University group following on from the January 24 report, and the first results of the modelling activity.

DESIGN OF THE STUDY

The objective of the 1996 activities was to continue the work undertaken in the Southern Ontario Oxidant Study (SONTOS). The aim of SONTOS is to obtain an improved understanding of the factors leading to elevated ozone concentrations in the Windsor Quebec corridor. The aim of the summer 1996 component of the project was to help characterise the emissions from the Greater Toronto Area (GTA), and to determine the composition of air masses that would travel down Lake Ontario and the St Lawrence River into Quebec. This was to be achieved by making measurements at the Binbrook site upwind of Hamilton and measurements from an aircraft upwind and downwind of Toronto.

A small aircraft was equipped with position, meteorological and chemical (NO₂, NO_x, and ozone) instrumentation, along with a system to fill canisters for subsequent laboratory analysis for hydrocarbons. The aircraft measurements were to be made under two meteorological conditions. The first was under south westerly flow, and the objective was to characterize the air masses leaving the GTA and moving downwind. The second was under clean northerly flow. The objective being to quantify the impact of emissions from the GTA.

INSTRUMENTATION AND METHODOLOGIES

The aircraft, a twin engine Piper Seminole, carried out in-situ measurements for ozone, NO₂, NO_x, temperature, and collected hydrocarbon samples in stainless steel canisters. Air was sampled from a point 80 cm aft of the nose of the aircraft, and 15 cm from the fuselage through individual 6.3 mm tubes, oriented perpendicular to the fuselage. Teflon tubing was used for the analysers and stainless steel for the hydrocarbon sampling.

Ozone and the NO_x species were measured using Scintrex-Unisearch Luminox7 Chemiluminescent analysers. Ozone was measured by a LOZ-3 O₃ (Eosin-y) analyser. The LOZ-3 data are corrected for pressure and temperature by the instrument itself. The LOZ-3 O₃ was calibrated by comparison to a Dasibi model 1003-AH ozone monitor. Two LMA-3 NO₂ luminol based analysers were also flown. The first measured NO₂ directly while the second sampled the air via a Permapur Nafion drier and CrO₃ NO to NO₂ converter (Drummond et. al 1990), to measure NO_x. The LMA-3 data were corrected for ambient pressure and non-linearity as described in Drummond et. al. 1990. The LMA3's were calibrated and zero checked before, after, and during each flight by an on-board permeation tube calibration system. The instruments were also audited by the Ontario Ministry of the Environment and Energy audit group, before and after the flight campaign, and no anomalies were observed. The air temperature was measured by using a thermistor located at the sample inlet, ambient pressure using a Sensym LX1602A and aircraft position by by Rockwell International model NavCorV GPS. Altitude was determined by the average of GPS altitude and the on-board pressure-altitude sensor.

DATA ANALYSIS ACTIVITIES

This activity has been concerned primarily with the aircraft data. We have now produced a compilation of all the data collected from the aircraft. The following table lists for the flights where reliable data were obtained, the flight times and the type of flow encountered.

Flight Dates	Flight Names	Flight Times	Type of Flow
July 10	1T	14:00-15:30	NNW
	1R	16:20-18:00	NNW
August 6	2T	14:15-16:30	S
	2R	17:00-18:30	S
August 18	4T	14:00-15:30	NW
	4R	16:15-18:00	W
August 24	5T	11:30-13:15	NW
	5R	14:00-16:10	N
August 29	6T	11:30-13:30	N
	6R	14:50-17:00	N

Appendix 1 contains: maps showing the flight track and ozone concentrations for the 9 successful flights; time serves for altitude, O₃, NO_x, NO₂ and time of hydrocarbon sampling and; Hydrocarbon concentrations determined for each of the canisters filled on these flights. The interpretation of these data along with the Binbrook measurements is proceeding.

One of the objectives of this study was to use these measurements and the photochemical criteria model to quantify or test our knowledge of the emissions from the Greater Toronto area. The methodology proposed was to use measurements made upwind of Toronto to initialize the model and to use the downwind measurements to test the model output, primarily governed by the emission inventory. Flights 4, 5, and 6 were all undertaken under north westerly flow and measurements were taken on flights perpendicular to the flow upwind and downwind of the city. We have used the data from these flights to produce contour maps of the ozone and NO₂ concentrations upwind and downwind of the city. These are presented in Appendix 2. The location of the hydrocarbon sampling are shown by the canister number on these plots, as are the location of the measurements used to generate the contours. Although the data coverage is less than would be optimum, it is clear that the concentration distribution is surprisingly homogeneous horizontally even downwind of Toronto. Thus, these data are appropriate for the analysis proposed.

We have begun a model study of Flights 5T and 5R on August 24 1996 aimed at investigating the emissions from the GTA.

CASE STUDY: August 24, 1996

The aircraft made several east-west legs approximately 60 km north of the Lake Ontario shoreline at Toronto between 11:30 and 12:30 EST. Altitudes were generally between 500m and 1000m with one spiral up to 3000m. Between approximately 2:30 and 3:30 EST downwind measurements were made in a south-west to north-east direction just offshore of Toronto. During this portion of the flight the aircraft altitude varied between 200m and 2000m.

Synoptic conditions for this period are presented in Figures 1 - 3 below. At 00Z August 23 (Figure 1) the synoptic flow over southern Ontario was from the south-west, in advance of a cold front that lay across the northern portion of Lake Huron. By 00Z August 24 (Figure 2) the cold front had moved to lie along the east coast of the United States and flow over southern Ontario was

from the north-west. A high pressure system centered over Minnesota at 00Z August 24, moved to lie just south of the Great Lakes by 00Z August 25 (Figure 3).

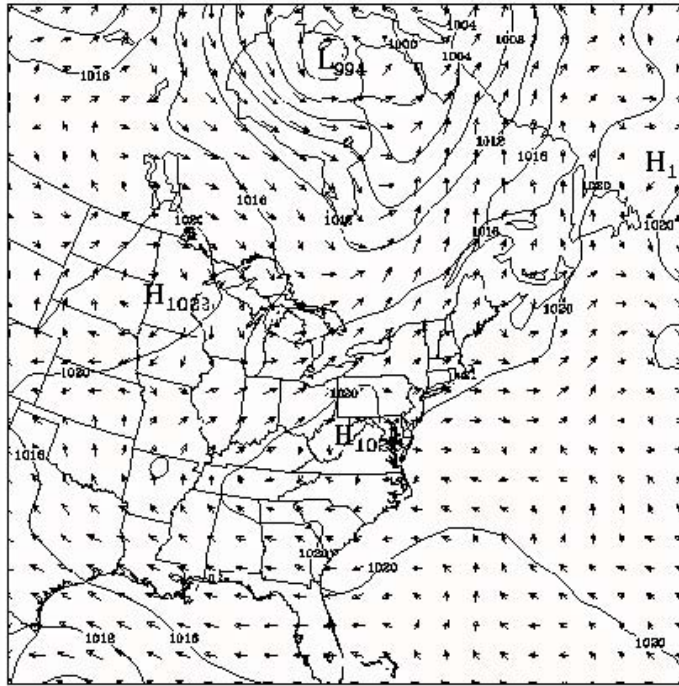


Figure 1: Surface pressure and 925 mb winds at 00Z August 23, 1996

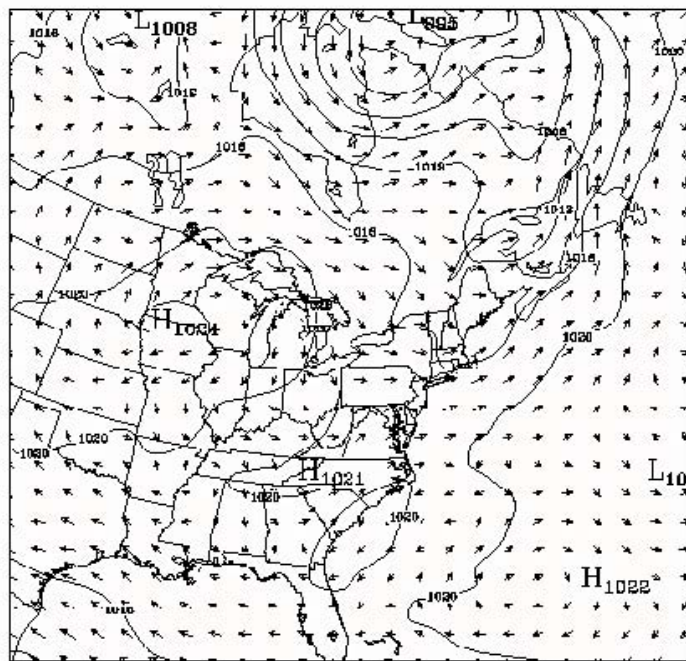


Figure 2: Surface pressure and 925 mb winds at 00Z August 24, 1996

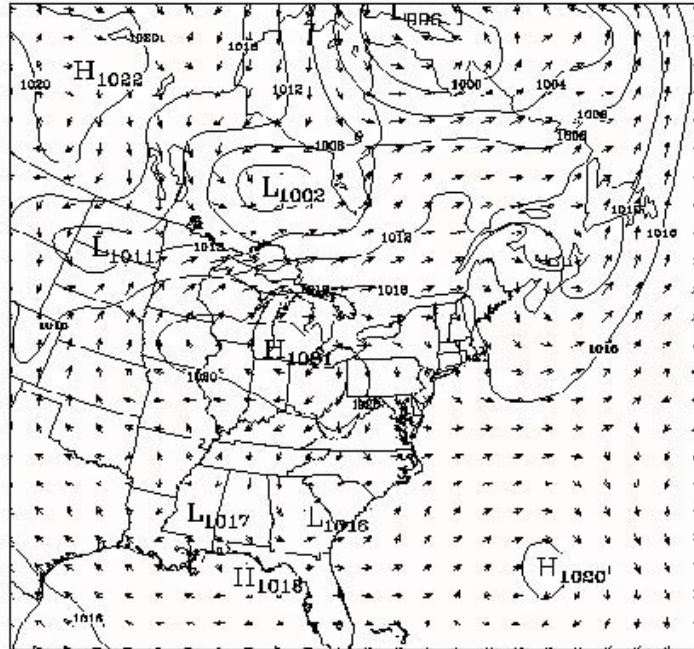
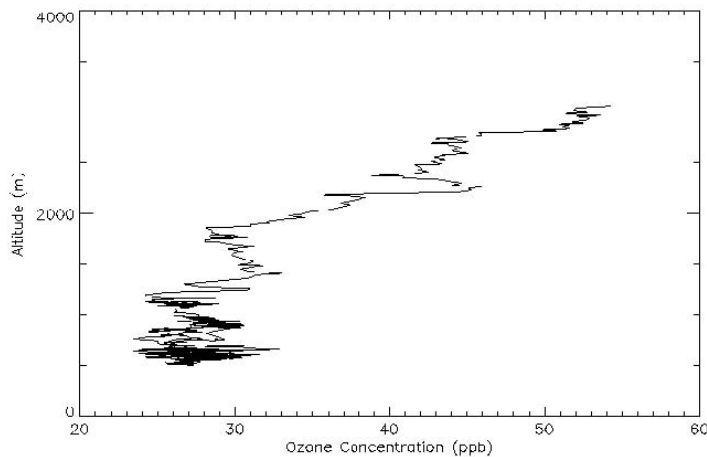


Figure 3: Surface pressure and 925 mb winds at 00Z August 25, 1996

Though back trajectories have not been computed for this day it is clear from the synoptic flow that the air mass over southern Ontario on August 24 had originated from the north-west. The aircraft observations of ozone, shown in Figure 4, give O₃ concentrations of approximately 30 ppb within the lowest 2.0 km, which is a typical ozone concentration within background

Figure 4: Aircraft observed O₃ concentrations vs. height for the upwind of Toronto flight



tropospheric air. It is interesting to note that ozone concentrations are considerably higher above 2.0 km, with a peak of over 50 ppb at 3.0 km. At this moment no explanation for this feature can be offered.

Figure 5 shows the observed NO_2 concentrations for the upwind of Toronto portion of the flight. Concentrations below a height of 1.0 km are generally between 1.5 ppb and 2.0 ppb. These levels of NO_2 may be the result of local emissions into an approximately 1.0 km deep boundary layer. The observed levels of NO_2 above 1.0 km are more problematic. The observations are showing between 0.5 ppb and 1.5 ppb of NO_2 up to a height of 3.0 km. It seems unlikely that local emissions and vertical mixing were sufficient to bring such a quantity of NO_x from the surface up to 3.0 km. Given the relatively short photochemical lifetime of NO_x (typically one day) and the fact that winds were from the north-west during this period a possible source for the observed levels of NO_2 is at this moment not known.

While observations of NO_2 and O_3 show some interesting, even perplexing, features above 2 km, the air within the planetary boundary layer seems to be characteristic of a background continental airmass. The higher concentrations of NO_2 within the boundary layer indicates that anthropogenic emissions to the north of Toronto are beginning to influence the chemical characteristics of the airmass, though the low levels of O_3 indicate that this influence has not been long-lived.

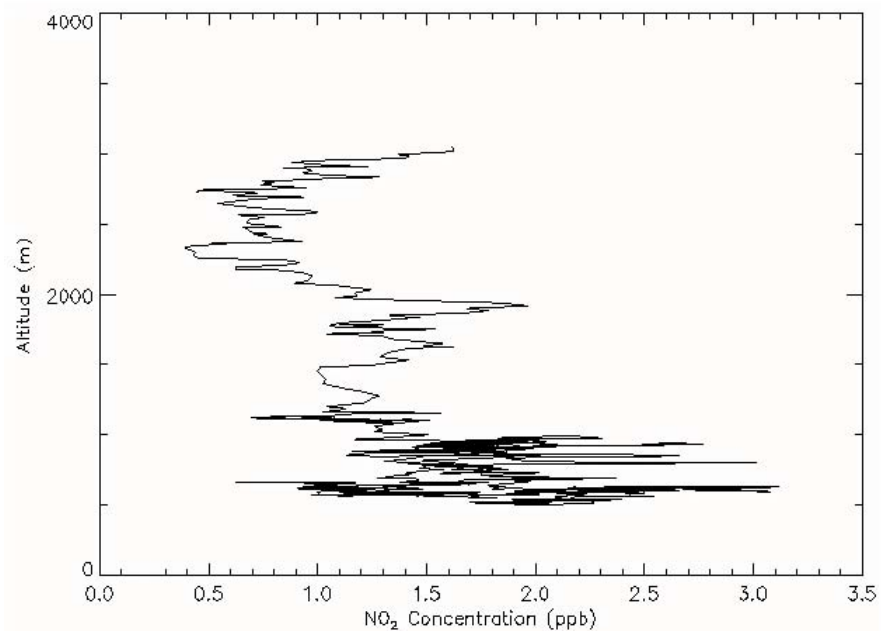


Figure 5: Aircraft observed NO_2 concentrations vs. height for the upwind of Toronto flight

The observations of NO_2 , O_3 , and hydrocarbons have been used to provide the boundary and initial conditions for a photochemical model that is being developed at York University. Boundary and initial conditions for species that were not measured were taken from an earlier model run on a larger, regional scale domain for similar meteorological conditions. The model has been run for August 24, 1996 and a comparison of the model calculated concentrations of O_3 , NO_2 , and hydrocarbons with the aircraft observations have been performed.

MODEL DESCRIPTION

The photochemical model used in this study is based on the Mesoscale Compressible Community model (MC2), a fully compressible model based on the semi-Lagrangian, semi-implicit method of Robert et al. (1985). The formulation of the numerical integration is quite efficient allowing for the use of comparatively long time-steps (Tanguay et al., 1990). Physical parameterizations of sub-grid scale processes, including the boundary layer and convection, are taken from the unified Recherche en Prevision Numerique (RPN) physics library (Mailhot et al., 1995).

Chemistry is calculated on-line with the meteorology through the addition of modules to the MC2 model to calculate emissions, dry deposition, chemical reaction and photolysis rates, and solve the chemistry. At present the chemical mechanism used is the Acid Deposition and Oxidants Model (ADOM) gas phase reaction set: wet chemistry is not included. Chemistry is calculated on each vertical level of the meteorological model and species are transported using the three-dimensional semi-lagrangian advection scheme native to the MC2 model. Dry deposition velocities are calculated using a resistance analogy in a similar way to that done within the ADOM model (Padro et al., 1993). Cloud effects on photolysis rates are calculated, again in a way that follows the original ADOM approach. Elevated major point sources are included, however presently there are no plume rise calculations performed and the emissions enter the model at the stack height.

The MC2 model has the ability to perform one-way nesting and this nesting capability has been extended to the trace species allowing high resolution simulations using boundary conditions provided by a more coarse resolution run. In a typical application of the model an initial run, with a domain covering much of the northeastern United States and adjacent regions of Canada, is performed. The chemical initial and boundary conditions for the coarse resolution run are interpolated from a global chemical transport model (McConnell et al., 1995). Boundary conditions for the meteorology are taken from objective analysis. The coarse resolution run then provides initial and boundary conditions for a finer horizontal resolution run focused on the region of interest.

The approach to using the model for this study has been slightly different than that discussed above. A version of MC2 without chemistry was run to develop meteorological initial and boundary conditions for the fine scale model run. This process involved running the meteorological model at two different horizontal resolutions; a 75 km horizontal resolution run on a 90 x 90 grid covering much of North America was performed to develop the synoptic scale flow, then a 21 km resolution run was performed, nested inside the original 75 km resolution run, focusing on the northeastern United States and southern Ontario. The grids used for these two runs are shown in Figure 6. The 75 km resolution run was 24 hours long, starting at 00Z July 24, 1996, and used the Canadian Meteorological Centre (CMC) objective analysis on sigma levels to provide initial and boundary conditions. The 21 km resolution run was started at 03Z July 24 and continued for 21 hours. These runs provided the meteorological boundary conditions for a 5.3 km resolution run of the full photochemical model focused on southeastern Ontario. All three of the model runs were made on the same vertical grid with 25 levels up to a height of 20 km, where 15 of these levels were located below 2.5 km.



Figure 6: Geographic extent of the 75 km and 21 km model grids.

Boundary and initial conditions for many of the chemical species were taken from an earlier model run for July 31, 1988. The meteorology on this day was quite similar to that of August 24, 1996. A cold front passed through southern Ontario late on July 30, and the synoptic flow on July 31 was from the northwest. Therefore it can be reasonably expected that both July 31, 1988 and August 24, 1996 were days when the chemical composition of the airmass entering southern Ontario was typical of background tropospheric air. An exception to the above was made for those species for which aircraft observations existed. For O_3 and NO_2 the initial and boundary conditions were set equal to the concentrations observed by the aircraft with a coarse representation of the variation of these concentrations with height. Since the model extended up to 20 km, the concentrations of O_3 and NO_2 were assumed to be constant with height above 3.0 km. While this is without a doubt a poor assumption, the size of the model domain is small enough to prevent the vertical transport of much of the material above 3 km down into the boundary layer. The concentration of NO was assumed to be 50% of the observed NO_2 concentration. Initial and boundary conditions for the hydrocarbon species were assumed to be constant everywhere and were set to the average concentrations found in the six hydrocarbon canister samples taken during the upwind flight.

The 5.3 km resolution model run was started at 12Z on August 24, and run for 12 hours. Anthropogenic emissions data is taken from the NAPAP 1985 inventory and, since August 24, 1996 was a Saturday, generic Saturday emissions for both area and major point sources were used. The area emissions (including mobile, non-mobile, and minor point sources) for the fine scale run were projected from the 21.167 km resolution emission database onto the 5.3 km model grid. No interpolation of the actual emission values were done. Rather all $16, 5.3 \times 5.3 \text{ km}^2$ grid squares that comprised a $21.167 \times 21.167 \text{ km}^2$ emission grid square took the value of the larger grid square, where the units of emission were normalized to a unit area. In this way the geographic distribution and total mass of emissions within the 21.167 km resolution database was preserved on going to the 5.3 km resolution model grid. This process did lead to the development of some problems. The 21.167 km grid shows considerable emissions present over the surface of the lakes. When the model was run with no modifications to the spatial distribution of the emissions very high concentrations of hydrocarbons and NO_x formed over the lake. In some places quite large emissions were specified to occur well out onto Lake Ontario and these

emissions were then being trapped within a shallow layer, due to the conduction inversion present within the model over the lake surface. To correct this problem, where a $21.167 \times 21.167 \text{ km}^2$ grid square was partially over water and was projected onto a $5.3 \times 5.3 \text{ km}^2$ grid square that was over water, the emissions from that $5.3 \times 5.3 \text{ km}^2$ grid square was equally distributed over the $5.3 \times 5.3 \text{ km}^2$ grid squares over land, but still within the same $21.167 \times 21.167 \text{ km}^2$ square. This process leads to no change in the spatial distribution of emissions as seen at a resolution of 21.167 km .

Unfortunately there were still three $21.167 \times 21.167 \text{ km}^2$ grid squares which were completely over water and with substantially higher emissions than surrounding regions. These grid squares were moved on to the nearest 21.167 km grid that was at least partially over land and then the process described above was performed to move the emissions completely over a land surface. For several $21.167 \times 21.167 \text{ km}^2$ grid squares completely over water, but with emission rates representative of rural regions the emissions were simply zeroed. It was felt that as a whole this process would avoid the unacceptable situation of having strong emissions into a lake based conduction inversion while leading to the minimum amount of distortion of the original emissions fields.

RESULTS

The wind speed predicted by the model over Toronto will have an important influence on the concentrations of precursors downwind of Toronto. When winds are light a particular air parcel will take a longer time to travel across the city. Figure 7 shows a comparison of the model predicted 10m winds and wind direction with hourly observations from Toronto International Airport. Both the model wind direction and speed show good agreement with the observations, though the model seems to predict a considerably higher than observed wind speed through the afternoon hours.

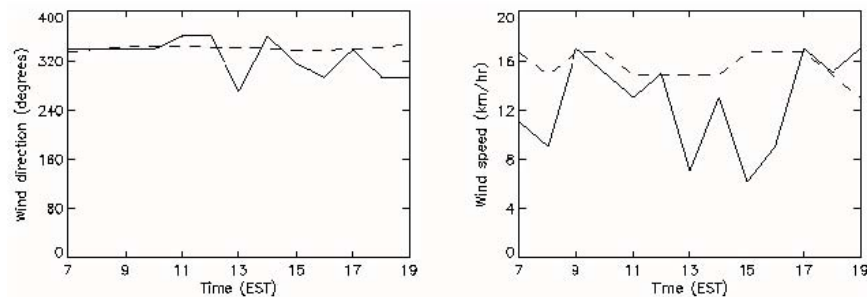
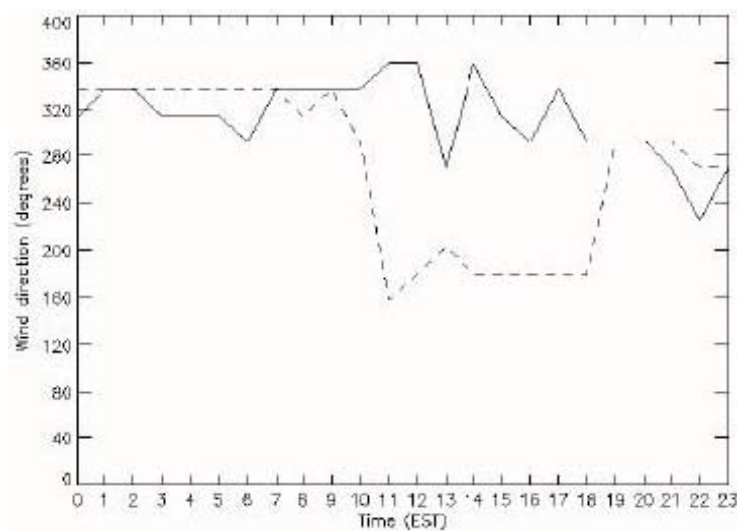


Figure 7: A comparison of the observed wind direction and speed at Toronto International Airport (solid lines) with the model calculated 10 m wind direction and speed (dashed lines) from 7:00 AM to 7:00 PM EST, August 24, 1996.

Comparing the observed wind direction at the Toronto International Airport with that observed by an automated station on Toronto Island (Figure 8) clearly shows the formation of a lake breeze on this day. Between 11:00 AM and 6:00 PM EST the wind direction at Toronto Island switches from the north-west to the south while the wind remains out of the north-west at the International Airport. Whether the perturbation of the pressure field that lead to the change

in wind direction at Toronto Island might also have lead to a weakening of the wind observed at the International Airport is not known at this time. Though it is interesting to note that the wind speed predicted by MC2 comes into better agreement with observations at the International Airport later in the evening after the lake breeze is observed to weaken.

While the MC2 wind field shows the dominance of the north-westerly synoptic flow, a weak mesoscale high is seen to form over the western end of Lake Ontario during the afternoon hours. The lake breeze predicted by the model does not penetrate far enough to the north and Figure 8: The observed wind direction at the Toronto International Airport (solid line) and at Toronto Island (dashed line) between 12:00 AM and 11:00 PM EST, August 24, 1996 Figure 8: The observed wind direction at the Toronto International Airport (solid line) and at Toronto Island (dashed line) between 12:00 AM and 11:00 PM EST, August 24, 1996



remains offshore. Though there is a band of southerly winds over the lake south of Toronto which agrees, at least qualitatively, with the observations at Toronto Island.

A comparison of the model predicted near-surface temperature with hourly observations recorded at the Toronto International Airport, shown in Figure 9, suggests that MC2 under-predicts the afternoon maximum temperature. A comparison of MC2 predicted temperatures with observations at other stations within southern Ontario for this date reveals a similar trend of under-predicting the maximum temperature by 1 or 2 degrees Celsius.

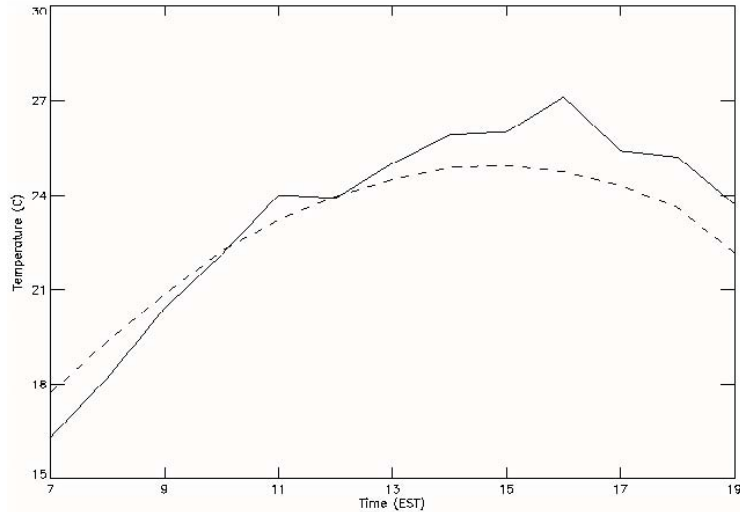


Figure 9: A comparison of the observed dry bulb temperature at Toronto International Airport (solid lines) with the model calculated temperature (dashed lines) from 7:00 AM to 7:00 PM EST, August 24, 1996.

The aircraft observations of NO_2 and O_3 downwind of Toronto have been compared with the model calculations of these species for the same region. Figure 10 shows the aircraft observations of the NO_2 concentration as a function of height and 10 different vertical profiles of NO_2 calculated by the model at 3:00 PM EST. The vertical profiles from the model were taken along a south-west to north-east line just offshore of Toronto and stretch across the entire width of the Toronto plume. These profiles provide a representative cross-section of the Toronto plume as it is calculated by the model. The aircraft observations show considerably enhancement of the NO_2 concentration below approximately 1.5 km. The comparison of measured NO_2 concentrations with the model show that the model is quite significantly under-predicting the concentrations of NO_2 leaving Toronto. Possible reasons include the strong temporal variation of major point sources that contribute a sizable fraction of the total NO_x emissions within Toronto. If possible these runs might be repeated with day specific emissions data for some of the major point sources within Toronto. Another possible explanation could be the NO_x chemistry within the model. Oxidation of NO_x to nitric acid occurs quite rapidly and model chemistry may be oxidizing the NO_x too rapidly. A more robust comparison of the model with observations would be to compare the total reactive nitrogen (NO_y) within the model with similar measurements.

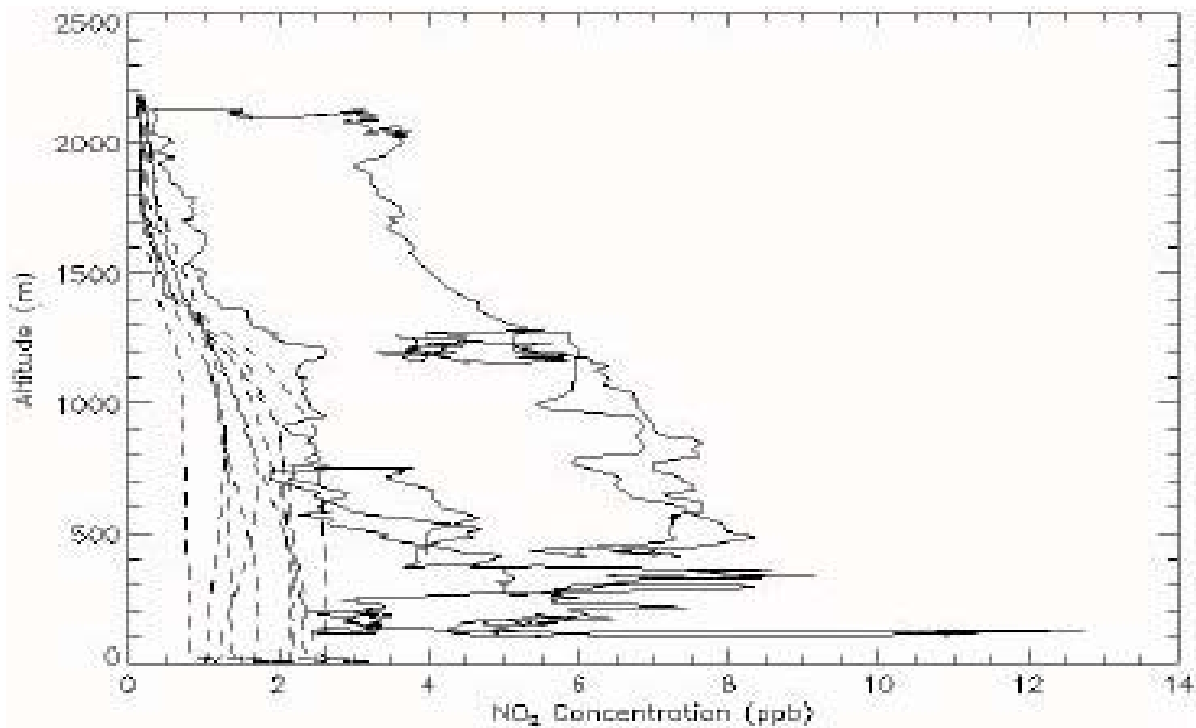
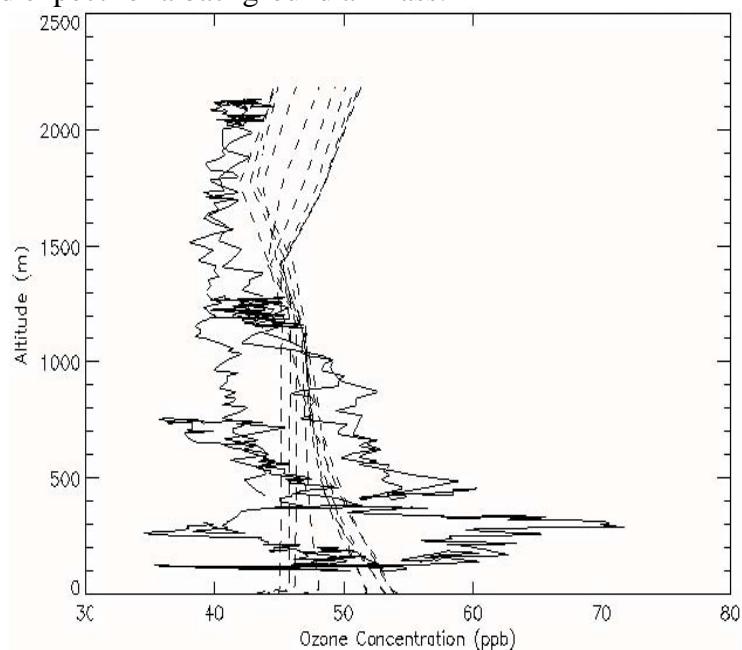


Figure 11 shows a similar comparison between aircraft observations and model calculations for ozone. Ozone concentrations show some under-prediction of the concentrations, especially below 500m. The over-prediction of ozone above 1.5km is related to the boundary conditions for O₃, which were based on the upwind of Toronto observations made earlier in the day. These observations (see Figure 4) showed considerably higher O₃ concentrations above 2.0 km. The downwind of Toronto concentrations of O₃ above the boundary layer are more in line with what one would expect for a background air mass.



A comparison of the downwind hydrocarbon data with the average downwind hydrocarbon concentrations has been performed. The results of this comparison are summarized below. Of the seven hydrocarbon canisters that were collected during the downwind of Toronto flight, six have been used in the calculation of the average downwind hydrocarbon concentration. The one canister that has been left out of this analysis was collected at a height of 2.1 km and shows considerably lower hydrocarbon concentrations than the other six. It seems likely that this sample was taken above the boundary layer and therefore does not strongly reflect any effects of emissions from Toronto.

The average modelled concentration was derived by calculating the average hydrocarbon concentration between the surface and 910m along the same series of 10 model columns used in the comparison of NO₂ and O₃ shown above. Since many of the hydrocarbon classes are quite reactive the rate at which vertical mixing occurs within the model will have considerably effect on the concentration of these species aloft. To give some idea of how the concentration of species varies vertically the average concentration of each hydrocarbon class within the 10 model columns was calculated at both 910 m and 60 m. The ratio of the average concentration at 60m to the average concentration at 910 m is given in the table as $[HC]_{60m}/[HC]_{910m}$. A coarse comparison of the model hydrocarbons with the observations show that the average hydrocarbon concentrations within the model are consistently at least a factor of two smaller than the aircraft observations. This inconsistency between the model and observations is not strictly a result of poor vertical mixing since the vertical variation in hydrocarbon concentration is considerably smaller than the difference between the model and observations.

Hydrocarbon Class	Average Measured Concentration (ppb)	Average Modelled Concentration (ppb)	Ratio $[HC]_{60m}/[HC]_{910m}$
Propane	0.8187	0.4053	1.196
Alkane	2.1467	1.1247	1.572
Ethene	0.3737	0.2081	1.470
Alkene	0.1407	0.0630	1.403
Toluene	0.3524	0.1173	1.540
Aromatics	0.1584	0.0778	1.497

Table 1. A comparison of the observed and modelled hydrocarbon concentration downwind of Toronto.

An explanation for the differences between the observed and model concentrations may in part be related to the too rapid oxidation of hydrocarbons within the model. Though the difference between the observations and the model seem to be much too large to be related to chemistry. Especially when one considers that the reactivity of the hydrocarbon classes within the ADOM chemistry have been tuned for the study of multi-day regional scale events and probably underestimates the hydrocarbon reactivity close to a large urban area.

The depth of the boundary layer predicted by the model will also have considerably effects

on how much dilution occurs due to vertical mixing of the emissions. Judging from the vertical profiles of NO₂ shown above it seems unlikely that MC2 is predicting a too deep boundary layer. In fact it appears from the NO₂ profiles that MC2 may be predicting a boundary layer that is slightly too shallow, though the differences do not appear to be large. A more shallow boundary layer would lead to higher concentrations of trace species as less vertical dilution would occur.

While the NO₂ measurements are continuous, hydrocarbon samples are only point measurements. Though six hydrocarbon samples have been used for the comparison with the model, there is a possibility that the hydrocarbon measurements do not represent the 'true' average concentration within the Toronto plume. Another open question at this moment is the degree to which the resolution of the emissions inventory leads to a Toronto plume that is too wide and too dilute. The comparison that has been made so far is between observed species concentrations and model calculated concentrations, and we are attempting to extrapolate this comparison to the emissions. The underlying assumption is that the volume into which these emissions are diluted is properly simulated within the model. In a similar way to which a too deep model boundary layer could lead to concentrations that are too low, a situation in which the emissions used by the model are artificially dispersed in the horizontal would also lead to modelled concentrations downwind of Toronto that are too low. It is hoped that further analysis of this case, as well as a similar comparison of model output with aircraft observations for other days will lead to a resolution of some of these uncertainties and a better estimate of the correct emissions for the Toronto region.

CONCLUSION

A preliminary comparison of modelled and observed concentrations for hydrocarbons and NO₂ has been shown. It appears that the model significantly underestimates the concentrations of both NO₂ and the hydrocarbons just downwind of Toronto. To what extent these differences are the result of inaccuracies in the model meteorology and chemistry and to what extent these differences are a reflection of problems with the emissions inventory is not clear at this moment. Though the differences in hydrocarbons appears to be much too large to be attributed to anything other than an underestimation of the emission strength.

It should be kept in mind that the emissions used for this study are generic Saturday emissions, as the day on which the measurements were made was also a Saturday. A similar comparison of model output and observations for a weekday would be valuable, and is planned for the near future. Day specific emissions for the major point sources may lead to considerable improvement in the model results, especially for NO₂. It is hoped that some day specific emissions data, for at least a few of the large point sources within the Toronto region, can be included in later analyses. One should also keep in mind that the emissions used for this study are for the year 1985 while the case studied occurred in 1996.

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