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Approaches to Regional Oxidant Modeling of the Eastern U.S. as Part of the Lake Michigan Ozone Study

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BACKGROUND

The Lake Michigan Ozone Study (LMOS) conducted a massive field study during the summer of 1991 to collect sufficient meteorological and air quality data to support the application of air quality modeling to develop emission control strategies that demonstrate attainment of the ozone standard. The LMOS has developed a comprehensive state-of-science photochemical modeling system by adapting emissions, meteorological, and ozone air quality models to the Lake Michigan region. The LMOS photochemical modeling system is centered around the nested-grid version of the Urban Airshed Model (UAM-V).[1,2,3,4,5] The UAM-V incorporates the latest treatments of two-way interactive grid nesting and subgrid-scale plume algorithms. Four ozone episodes from the 1991 field study have been selected for simulation:

Episode 1: June 26-28, 1991
Episode 2: July 17-19, 1991
Episode 3: August 25-26, 1991
Episode 4: June 20-21, 1991

The UAM-V is exercised for two days proceeding each episode as an initialization period designed to eliminate the influence of boundary conditions. LMOS episodes 1 and 2 occurred during the 1991 field study intensive periods; in addition to the enhanced continuous monitoring of the 1991 summer study special measurements were taken (e.g., aircraft observations and speciated hydrocarbon measurements) during intensive periods. LMOS episode 3 occurred after the summer field study; no intensive data existing and many of the enhanced continuous monitoring measurements were discontinued prior to the episode. The fourth LMOS episode took place during the 1991 field study but no intensive measurements were taken. Details of the 1991 LMOS field study are found elsewhere.[6]

LMOS AIRCRAFT MEASUREMENTS

During the LMOS intensive periods up to seven aircraft were in operation collecting air samples aloft. The standard five aircraft were always in operation during the intensive periods collecting measurements along the flight paths depicted in Figure 2. Two additional aircraft provided special study data; one mapping the vertical distribution of ozone using a downward looking differential absorption lidar (DIAL)[7], the other used as a backup aircraft and for tracer studies. The aircraft were operated by the North American Weather Consultants (NAWC), National Oceanic and Atmospheric Administration (NOAA), SRI international, and the Wisconsin Department of Natural Resources (WIDNR). The flight paths for the standard LMOS aircraft are given in Figure 1 with the definition of each aircraft as follows (details on the aircraft operations can be found elsewhere[8]):

LMOS 1:	Two dimensional data plane (2DDP) (NAWC)
LMOS 2:	Chicago Box (NAWC)
LMOS 3	Boundary Flight (NAWC)
LMOS 4:	Secondary 2DDP (NOAA)
LMOS 5:	DIAL (SRI)
LMOS 6:	Backup and Tracer Study (NAWC)

Each of the standard aircraft were equipped to measure ozone, NO/NO_x, temperature, hydrocarbons, carbonyls, and other parameters. The aircraft data have proven invaluable for both the rigorous evaluation of the ability of the UAM-V to predict the three-dimensional structure of ozone and ozone precursors within the Lake Michigan region, but also for identifying the importance of ozone transported from upwind regions into the Lake Michigan area and the adequacy of regional-scale ozone models for replicating such transport.

LMOS PHOTOCHEMICAL MODELING SYSTEM

The LMOS Photochemical Modeling System consists of three main models that provide inputs for the UAM-V (Figure 2).

GEMAP is an emissions model that can generate day-specific, gridded, speciated, hourly varying emission rates of NO_x, VOC, and CO.

CALRAMS is a nonhydrostatic prognostic meteorological model that provides representation of meteorological conditions, including the complex air flows due to the lake breeze systems.

ROM is a regional oxidant model that will provide initial concentrations and boundary conditions (i.e., transported pollutant concentrations) for the UAM-V.

For the LMOS study, the UAM-V was configured with three levels of nested grids as depicted in Figure 3. The emissions model (GEMAP) and meteorological model (CALRAMS) provide data at the 16, 8, or 4 km resolution required by each of the UAM-V's nested grids. The ROM model is configured with an 18.5 km horizontal grid and three vertical layers. This coarse resolution may be insufficient to properly simulate ozone formation over the midwestern U.S. and provide accurate estimates of boundary conditions for the UAM-V. ROM modeling activities are currently behind schedule; there is a possibility that the ROM simulations for the later LMOS episodes may not be performed. In addition, to evaluate future-year emission control strategies the Lake Michigan Ozone control Program (LMOP), the continuation of LMOS, will require future-year ROM simulations consistent with the emission control strategies under study. Since the meteorological conditions (CALRAMS) for the ozone episodes will remain fixed for the evaluation of future-year control strategies and LMOP will be operating the GEMAP to obtain emission inputs for the mesoscale application of the UAM-V (Figure 3), the future-year ROM simulations may become the critical element that would limit the LMOP and the identification of ozone attainment emission control strategies. For these reasons, the LMOS/LMOP decided to investigate the feasibility of performing regional-scale ozone simulations using the UAM-V to provide initial and boundary conditions for the more refined mesoscale application of the UAM-V in the Lake Michigan region. If the UAM-V regional-scale applications provides acceptable ozone estimates, then the LMOP could apply the UAM-V in the regional-scale mode to provide initial and boundary conditions for the mesoscale UAM-V application and not be limited to only those emission scenarios and future-years for which ROM simulations are available.

APPROACH TO UAM-V REGIONAL-SCALE MODELING

At this time the EPA Regional Oxidant Model (ROM) has been exercised over the eastern U.S. for the first two LMOS episodes using two different sets of meteorological inputs: (1) meteorological inputs based on interpolating surface and upper-air meteorological observations

(McIdas data) to the ROM grid using the ROM meteorological preprocessor[9]; and (2) meteorological inputs derived from the CALRAMS simulation. For the ROM/CALRAMS meteorological inputs, each of the CALRAMS 80 km grid hourly prognostic model estimates were treated like a surface and upper-air meteorological measurement in the ROM meteorological preprocessor.[9] As the ROM has already been setup for the first two LMOS episodes, if the UAM-V is to be used for regional-scale modeling in subsequent LMOS episodes, the differences between the ROM and UAM-V, as applied on the regional-scale, need to be identified. Although the ROM vertical resolution is limited to three layers (based on the mixing height) and horizontal resolution is limited to approximately 18.5 km, the UAM-V has no such limitations. However, to compare the ROM and UAM-V the models must first be run in a consistent fashion so that the models, rather than the resolution, are being compared.

In the first regional-scale application of the UAM-V it will be configured with the exact same vertical (3 layers) and horizontal (18.5 km grids) resolution as the ROM. The ROM/CALRAMS LMOS episode 1 simulation meteorological, emissions, and initial and boundary condition inputs will be mapped to the UAM-V format and the UAM-V exercised for a UAM-V ROM emulation simulation. For the second UAM-V regional-scale simulation of LMOS episode 1, the same (ROM 18.5 km) horizontal grid will be used (so that emissions, initial concentrations, and boundary conditions can be kept the same), but the CALRAMS 80 km grid meteorological model estimates will be mapped directly to the UAM-V. In this application the UAM-V will use more vertical layers than ROM and the vertical layer structure will be consistent with that utilized by the CALRAMS (i.e., terrain following approximately spatially and diurnally constant), rather than spatially and diurnally varying tied to the mixing height. The two UAM-V regional-scale simulations will be compared to the ROM/CALRAMS estimates and with available observations. If the UAM-V regional-scale application is deemed adequate and provides useful information, it may be applied for other LMOS episodes. One of the key judgements of adequacy of the ROM and UAM-V regional-scale simulation is how it compares to the LMOS boundary aircraft observations (see Figure 1).

LMOS BOUNDARY AIRCRAFT OBSERVATIONS AND ROM

The LMOS boundary aircraft observations have been compared against the ROM estimates along the upwind portions of the flight path to evaluate the adequacy of using ROM estimates as boundary conditions for the UAM-V mesoscale domain (Figure 3). Initial comparisons identified that at night and early morning the ROM layer 3 estimates are essential identical to the top boundary conditions (40 ppb). Thus, the ROM/UAM-V initial and boundary condition processing program was modified to ignore ROM layer 3 estimates so that only ROM estimates in layers 1 and 2 were used, an approach similar to that utilized by the ROM/UAM interface program.[10] The ROM two-layer model estimates were then compared against the LMOS boundary aircraft observations to determine whether there were any bias in the ROM estimates, similar comparisons will be made with the UAM-V regional-scale application. Comparisons were made for ozone, NO_x, and reactive organic gases (ROG). However, because the aircraft NO_2 measurements also contain some PAN and nitric acid, the comparison of ROM estimates and measured odd nitrogen species is difficult. Furthermore, there were very few ROG grab samples collected along any aircraft flight, thus the comparisons for ROG are also not very rigorous. Thus, we focus on the comparison of ROM ozone estimates with ozone measured by the LMOS boundary aircraft to judge the adequacy of the ROM estimates for providing boundary conditions for the UAM-V.

During LMOS episodes 1 and 2, field study intensive periods occurred on June 25-27, 1991 and July 16-18, 1991 at which times the LMOS boundary aircraft conducted three flights a day; early morning, noon, and afternoon. Because the synoptic winds during LMOS episodes 1 and 2 were predominately from the south or southwest, the southern and western legs of the boundary aircraft are particularly important when compared to the ROM (or UAM-V regional) estimates (see Figure 1). Figures 4 through 6 display the boundary aircraft observed ozone and the concurrent ROM/McIdas estimated ozone along the southern and western legs of the LMOS boundary aircraft flight for the three flights on June 26, 1991. The results from other days are similar as well as, qualitatively, the ROM/CALRAMS ozone results. The ROM vertical cross sections were constructed using only ROM layers 1 and 2 estimates and assuming that the ROM concentration represented the centroid of the ROM grid cell.

Morning Flight

In the morning on June 26, 1991 along the LMOS southern boundary, observed ozone in the surface layer (below 300 m agl) varied from 20-50 ppb (Figure 4a). Observed ozone above the surface layer and below 1300 m agl was approximately 90 ppb in the western (87.7-89 degrees longitude), 70 ppb in the middle (86.3-87.7 degrees), and 80 ppb in the eastern (85-86.3 degrees) portions of the southern boundary flight. Concurrent ROM/McIdas estimates above the surface layer and below 1300 m for the same subregions were approximately 55 ppb (50-60 ppb), 60 ppb (55-70 ppb), and 60 ppb (55-65 ppb) (Figure 4b). Above 1300 m agl 68-78 ppb is observed at the western edge of the southern flight leg whereas the ROM estimates are 50-55 ppb (note that ROM layer 3 estimates (not shown) at 1700-1800 m agl were 42 ppb at this time.

Along the western boundary flight observed ozone out of the surface layer and below 1300 m agl are approximately 95 ppb (80-110 ppb) in the southern and 75 ppb (63-81 ppb) in the northern portions of the flight (Figure 5a). Concurrent ROM estimates in the southern and northern portions of the flight range from 45 to 60 ppb and 55 to 65 ppb, respectively (Figure 5b). Above 1300 m agl, the observations indicate an elevated ozone reservoir aloft in the 70-80 ppb range, whereas ROM estimates range from 45-65 ppb (again note that ROM layer 3 estimates at 1700-1800 m agl were an almost uniform 42 ppb).

In summary, the ROM ozone estimates above the surface layer (300 m agl) appear to be systematically underestimating the observed aircraft observations on the morning of June 26, 1991. This systematic underestimation ranges from 10 to 50 ppb. Above 1300 m agl, when ignoring ROM layer 3, the ROM underestimation appears to be in the 5-35 ppb range. If ROM layer 3 estimates are used, then the underestimation aloft ranges from 30-40 ppb.

Noon Flight

Around noon on June 26, 1991 the observed ozone along the southern leg of the LMOS boundary flight is fairly uniform both horizontally and vertically and ranged from 80 to 90 ppb (Figure 6a). ROM estimates at the same time and location range from 50 to 70 ppb and are also vertically uniform and horizontally fairly homogeneous (Figure 6b). Thus, it appears ROM underestimates the inflow ozone concentrations across the southern boundary by 10 to 40 ppb at around noon on June 26, 1991.

Along the western leg of the flight, the observed values are fairly uniform vertically but are approximately 85 ppb (78-94 ppb) in the southern and 75 ppb (69-85 ppb) in the northern portions of the flight (Figure 7a). ROM estimates in the southern and northern portions of the western leg of the flight are in the 66 to 80 ppb and 80 to 95 ppb range, respectively. Thus, at noon on June 26th along the western leg of the LMOS boundary flight the ROM tends to underestimate the observed ozone on the southern and overestimate the observed ozone on the northern portions of the flight.

Afternoon Flight

In the afternoon on June 26, 1991 observed ozone along the southern boundary range from 75 to 101 ppb, with approximately 90 ppb aloft in the western portion of the southern boundary (Figure 8a). Concurrent ROM estimates along the southern boundary flight range from 53 to 86 ppb (Figure 8b). Thus, on the afternoon of June 26th the ROM is underestimating the ozone along the southern boundary of the LMOS domain by 5-35 ppb.

The ROM does a better job in replicating the LMOS boundary aircraft ozone observations along the western leg of the June 26 afternoon flight; ROM estimates range from 55 to 85 ppb whereas the observed values range from 65 to 93 ppb. The ROM underestimation bias ranges from 0 to 20 ppb.

SUMMARY AND CONCLUSIONS

Ozone and ozone precursors transported from upwind regions influence the observed peak ozone concentrations in the Lake Michigan region. Sensitivity simulations indicate that any bias in the ozone boundary conditions (i.e., ozone transported from upwind regions) results in a similar bias in the estimated ozone in the Lake Michigan region. Comparison of aircraft observations from the LMOS boundary aircraft with ROM results indicate a 10 to 50 ppb bias toward underestimation of the observed ozone above the surface. Thus, using the ROM boundary conditions one would expect a similar underprediction of the peak ozone concentrations to occur in the Lake Michigan region.

The LMOS/LMOP is investigating alternative methodologies for defining concentrations of ozone and ozone precursors transported into the Lake Michigan region including an observational approach and applying UAM-V in a regional-scale mode. However, the observational approach is limited to estimating current year ozone concentrations. The UAM-V regional-scale applications may suffer from the same deficiencies (ozone underestimation) as the ROM simulations, which may point to fundamental problems with model inputs (e.g., and underestimated ROG inventory). However, with the regional-scale UAM-V the LMOS/LMOP can perform many additional simulations to investigate potential ozone underestimation problems and provide initial and boundary conditions for future-years under a variety of different regional emission control program scenarios.

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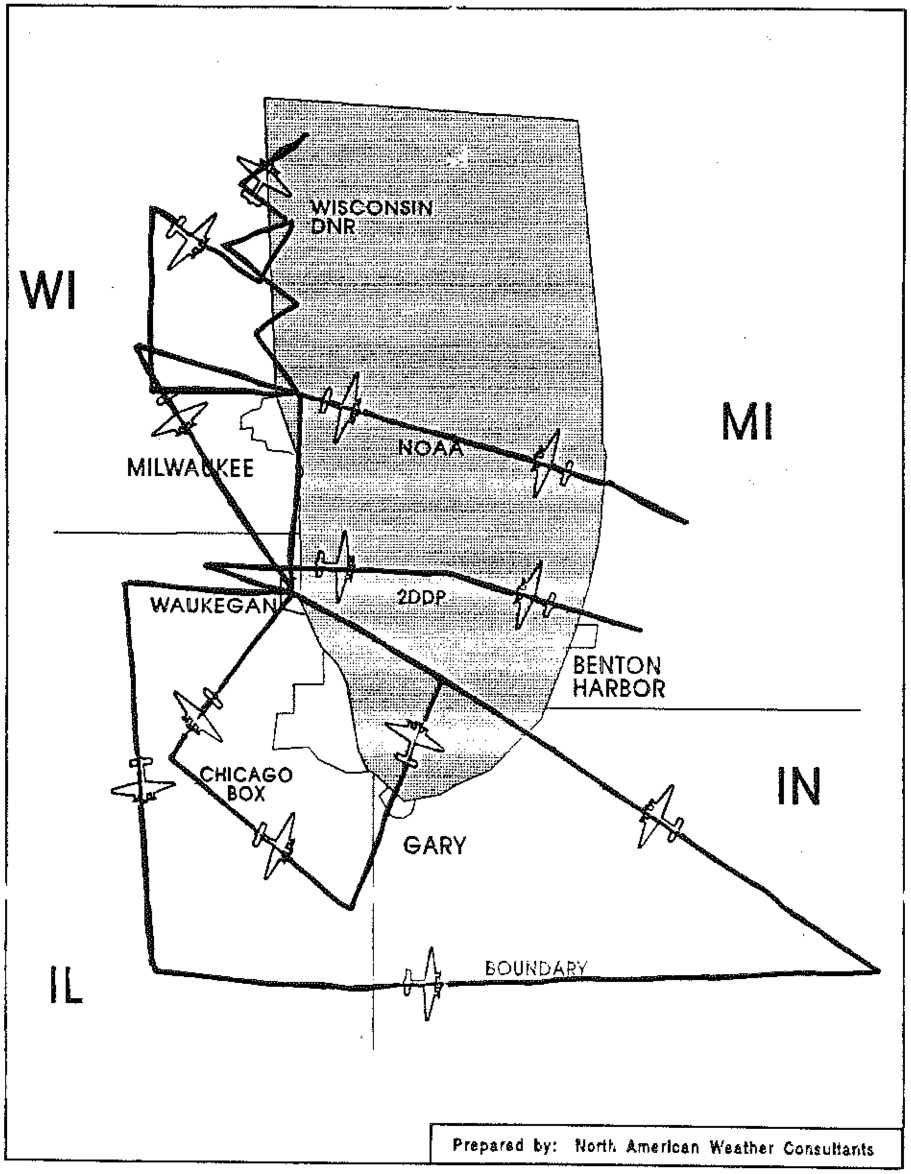


Figure 1. Flight paths of aircraft during the 1991 Lake Michigan Ozone Study (LMOS) intensive periods.

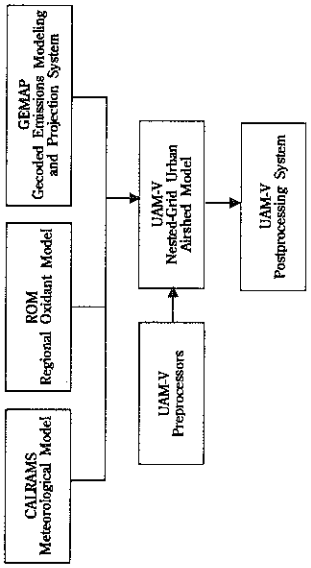


Figure 2. Structure of the LMOS photochemical modeling system.

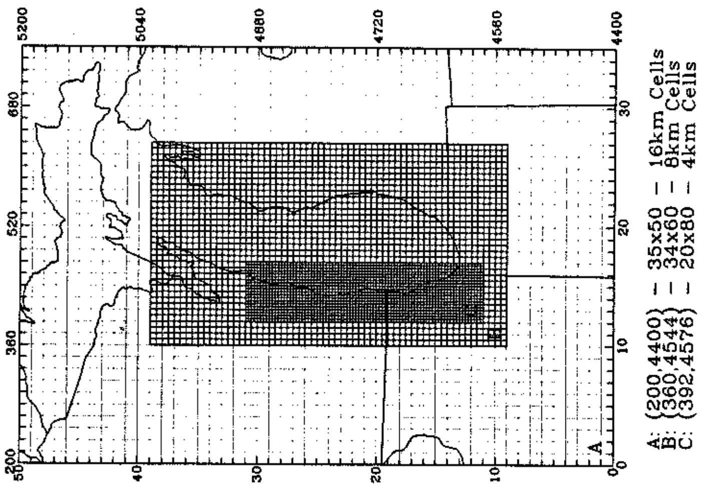
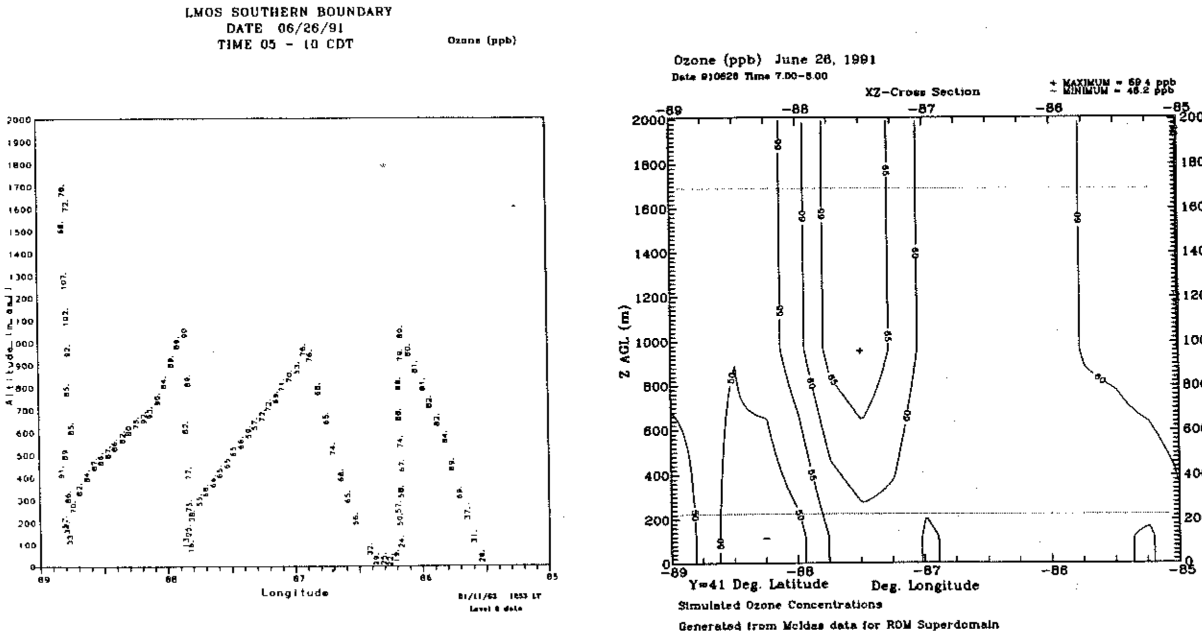


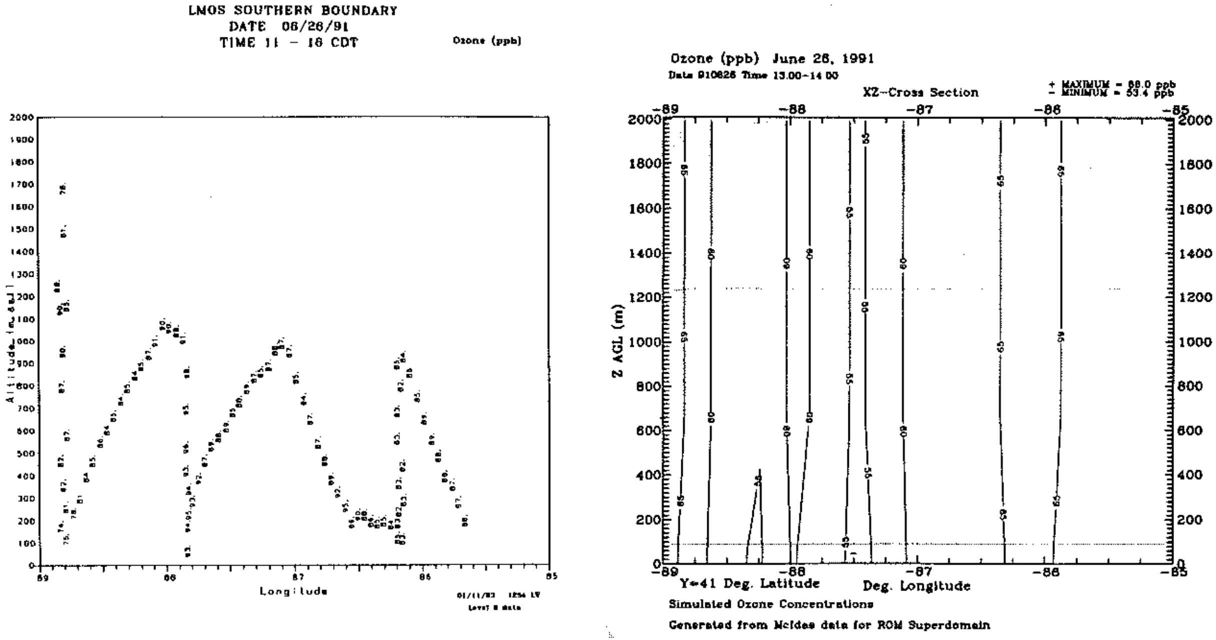
Figure 3. Nested-grid structure used in the mesoscale application of the UAM-V to the Lake Michigan region.



(a) Observed Ozone (ppb)

(b) ROM/McIdas Estimate Ozone (ppb)

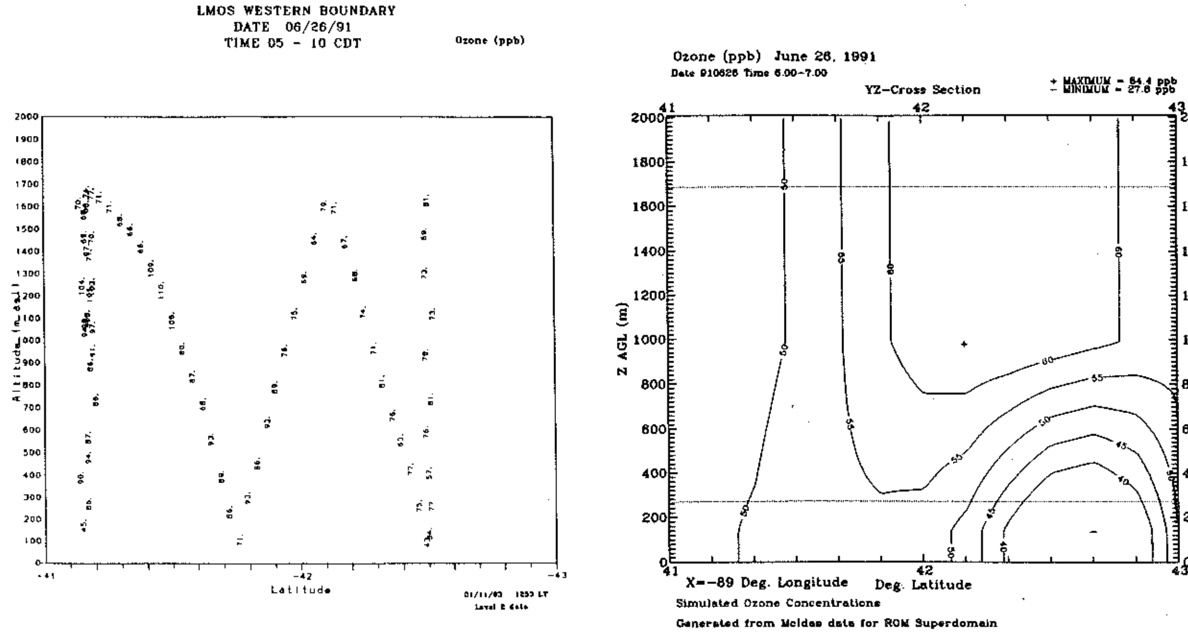
Figure 4. Observed and ROM/McIdas estimated ozone (ppb) along the southern leg of the LMOS boundary flight path in the early morning of June 26, 1991.



(a) Observed Ozone (ppb)

(b) ROM/McIdas Estimate Ozone (ppb)

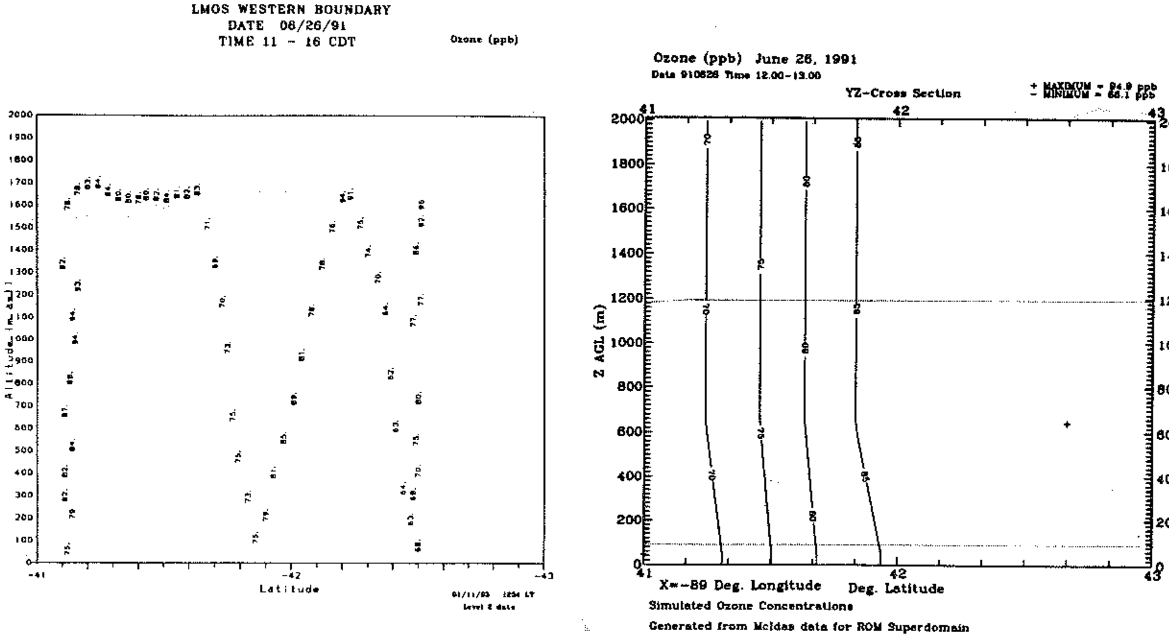
Figure 6. Observed and ROM/McIdas estimated ozone (ppb) along the southern leg of the LMOS boundary flight path at noon on June 26, 1991.



(a) Observed Ozone (ppb)

(b) ROM/McIdas Estimate Ozone (ppb)

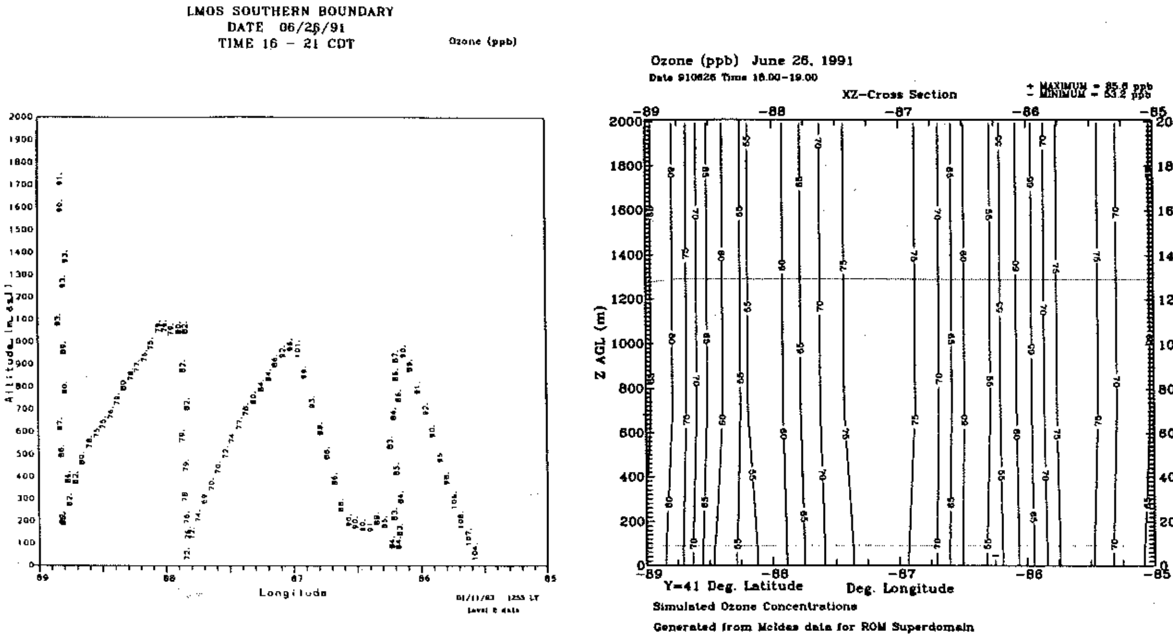
Figure 5. Observed and ROM/McIdas estimated ozone (ppb) along the western leg of the LMOS boundary flight path in the early morning of June 26, 1991.



(a) Observed Ozone (ppb)

(b) ROM/McIdas Estimate Ozone (ppb)

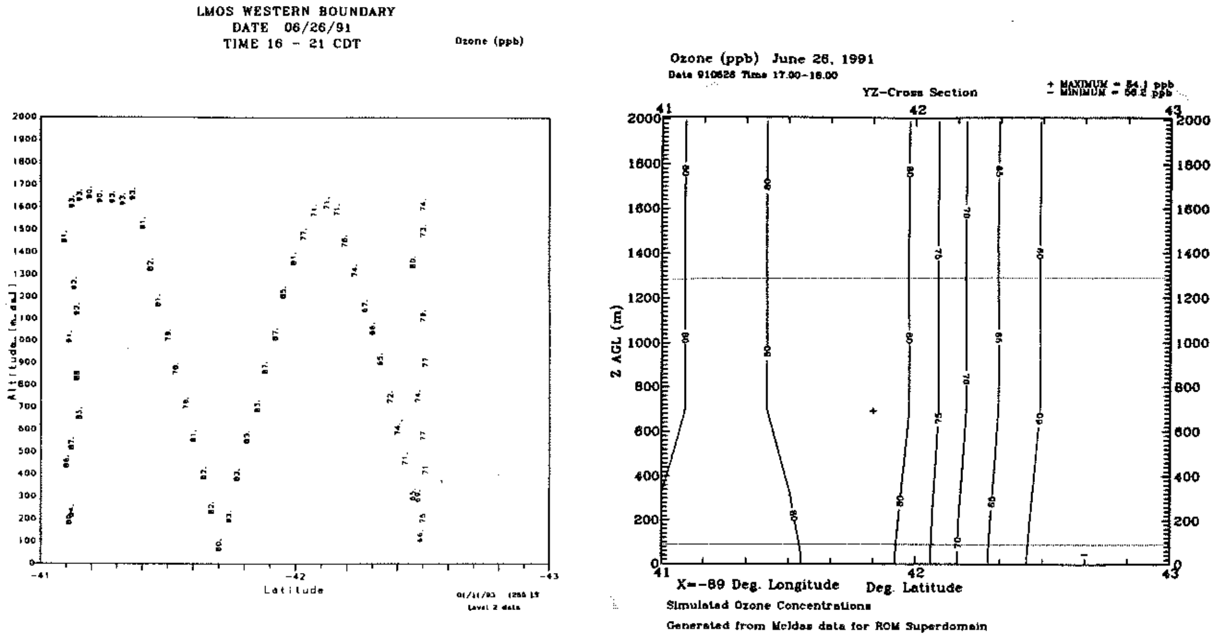
Figure 7. Observed and ROM/McIdas estimated ozone (ppb) along the western leg of the LMOS boundary flight path at noon on June 26, 1991.



(a) Observed Ozone (ppb)

(b) ROM/McIdas Estimate Ozone (ppb)

Figure 8. Observed and ROM/McIdas estimated ozone (ppb) along the southern leg of the LMOS boundary flight path in the afternoon of June 26, 1991.



(a) Observed Ozone (ppb)

(b) ROM/McIdas Estimate Ozone (ppb)

Figure 9. Observed and ROM/McIdas estimated ozone (ppb) along the western leg of the LMOS boundary flight path in the afternoon of June 26, 1991.