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Photochemical Modeling of the Lake Michigan Region Using the Nested-Grid Urban Airshed Model

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CALRAMS. For the first few vertical layers near the surface, the UAM-V utilizes the same layer depths as the CALRAMS and then combines two or more CALRAMS layers for one UAM-V layer near the top of the domain, resulting in eight total UAM-V vertical layers. The vertical diffusivities are not taken directly from CALRAMS output but are deduced for the UAM-V layer structure in each grid using the same formulas as in the CALRAMS.

Initial and Boundary Concentrations

The EPA ROM model is exercised on a domain larger than the LMOS modeling domain. Its results are then used to define initial concentrations and boundary conditions for the UAM-V, i.e., inflow concentrations along the boundary of the 16 km UAM-V grid (the region labeled "A" in Figure 1). The ROM is exercised for a multi-day period for a modeling domain covering the entire eastern U.S. The ROM utilizes a latitude/longitude grid system with a resolution of approximately 18 km. The ROM results are interpolated to the appropriate UTM grid points to define initial concentrations for all species. Likewise, concentrations are interpolated to each boundary point along the edge of the 16 km grid system. The resultant three-layer ROM concentrations are then mapped to the UAM-V eight-layer structure assuming column mass conservation.

Emissions Inputs

Emissions inputs for the UAM-V are supplied by the GEMAP emissions modeling system. Emissions for a typical summer weekday or weekend day are supplied on the UAM-V 16 km grid (region A in Figure 1) and day-specific emissions are supplied at a 4 km resolution for the UAM-V 8 km grid (the region labeled B in Figure 1). The 4 km gridded emissions data are aggregated to the 8 km grid; appropriate portions of the 4 km gridded emissions are used as is for the UAM-V 4 km grid (region C in Figure 1). In addition to the gridded low-level emissions data, GEMAP provides elevated point source data for each of the grids (regions A and B). Since point source locations in UAM-V are defined by UTM coordinates, only a single file of point source data is used. The point source files for regions A and B are therefore combined before exercising the UAM-V. Some sources in the region B file have to be excluded because they are physically located outside of region B. In addition, sources in the region A file that are also located within region B are excluded. The remaining sources are merged into a single point source input file for use by the UAM-V.

Other UAM-V Inputs

The fractions for each of 11 land cover types for each of the grid locations in the modeling region are input to the UAM-V. For the LMOS, digitized land use data at approximately one-quarter by one-sixth degree longitude/latitude, available from the US Geological Service, were used to specify land use fractions in the 16 km grid used by UAM-V. Subsequently, higher-resolution land use data became available and were used to develop land use data for both the 8 km and 4 km grids.

Based on published work in regional ozone modeling[5] and on other available data,[6,7] albedo data were derived from the land use data described above with the following correspondence:

Land Use Type	Albedo
Vegetation	0.05
Urban	0.08
Water	0.04

Turbidity was set to 0.094, a value representative of rural conditions. Ozone column data were obtained from the National Space Science Data Center (NSSDC), which derives estimates from the orbiting Total Ozone Monitoring Spectrometer (TOMS). The grid spacing for the daily average ozone column data used to develop UAM-V input data is 1° latitude by 1.25° longitude.

The range of values of albedo, turbidity, and ozone column was determined for the data being used for episode 1 (see below). Five values of albedo, three values of turbidity, and five values of ozone column were then selected to represent conditions in the modeling episode. For episode 1, the ozone column data values ranged from 304 to 356 Dobson units. Utilizing a photolysis rates preprocessor,[2] a table of photolysis rates was calculated for each of the combinations of these values covering 11 solar zenith angles ranging from 0. to 90. degrees and 11 altitudes ranging from 0. to 4,210 meters above mean sea level.

LMOS EPISODE 1

The LMOS photochemical modeling system was initially tested for an ozone episode from July 1987.[8] This preliminary model application was designed to test the data handling and model application techniques of the LMOS photochemical modeling system. Results of the preliminary application were encouraging; the model predicted the observed pattern of a sharp gradient of ozone concentrations from the lake leading inland.

The LMOS photochemical modeling system was then used to simulate the June 24-28, 1991 period, denoted as episode 1. The ROM and CALRAMS models have been exercised for a longer period and for a larger modeling domain than that used in the UAM-V to limit the influences of initial and boundary conditions on the UAM-V model calculations. The UAM-V simulation period was also extended to June 22, two days prior to the ozone episode, to limit the influence of the UAM-V initial concentrations, which were obtained from the ROM model estimates. To lower the computational requirements of extending the simulation period to the two initialization days, the model was run with only the coarse (16 km) grid spacing. In addition, most of the sensitivity simulations with UAM-V are being run with only the 16 km and 8 km grids and not the 4 km grid. The periods of simulations and grid spacing (km) for each of the components of the LMOS photochemical modeling system are given below.

Date	ROM	CALRAMS	GEMAP	UAM-V
June 22	18.5	80	--	--
23	18.5	80	--	--
24	18.5	80/16	16	16
25	18.5	80/16	16	16
26	18.5	80/16/4	16/4	16/8/(4)
27	18.5	80/16/4	16/4	16/8/(4)
28	18.5	80/16/4	16/4	16/8/(4)
29	18.5	80	--	--

In the initial UAM-V simulations of episode 1 the peak observed ozone values were considerably underpredicted. Although inaccuracies in any of the input data (meteorological, emissions, boundary and initial concentrations) could result in underprediction of ozone concentrations, we are focusing our initial investigation of the underprediction on boundary concentrations.

EVALUATION OF UAM-V BOUNDARY CONCENTRATIONS

Boundary concentrations for episode 1 are derived from ROM2.2 predictions using meteorological inputs derived from the McIdas observational data set. As part of the LMOS monitoring program, aircraft flights measuring ambient ozone and NO_x concentrations were made near the boundaries of the UAM-V modeling region during episode 1. It is therefore possible to make direct comparisons of the ROM predictions with observed data along vertical slices through the modeling region. Vertical slices of ROM2.2/McIdas and aircraft observations of ozone along the southern and western legs of the aircraft flight are shown in Figures 3 and 4. Because the aircraft NO_x instrument also picks up some of the PAN, HNO_3, and some other nitrogen compounds, evaluation of the ROM2.2 NO_x estimates against the aircraft data is somewhat ambiguous and will not be presented here. Comparisons are presented for the morning aircraft flight that took place on June 26, 1991.

The vertical slices of ROM2.2/McIdas concentration isopleths are based on the three layers of ROM estimates. To interpret the vertical isopleths of ROM concentrations correctly, one needs to consider two points. First, the concentrations in the third ROM layer are extrapolated to the top of the plot; thus ROM results actually end at the top of the third layer (the top of each layer is indicated by a dashed line in Figure 3a). Second, the concentrations in each ROM layer are assumed to represent the mid-point of the layer; the isopleth interpolation plotting program interpolates between these data to draw the isopleths. The same scale was used in plotting the vertical ROM/McIdas concentration estimates and aircraft observations to facilitate comparison; much of the analysis described in the following paragraphs was obtained by superimposing transparencies of the aircraft observations on the vertical ROM estimates.

In the western section (−89 to −88 longitude) along the southern boundary on the morning of June 26 the ROM2.2/McIdas ozone concentrations underestimate the observed values from the aircraft above the surface layer by about 30 - 55 ppb (85 - 107 ppb observed versus 40 - 57 ppb estimated). In the center (−87 longitude) the ROM2.2/McIdas concentrations exhibit almost no bias between 300 - 1000 m above ground level. In the eastern section (−86 to −85 longitude) they tend to underpredict the aircraft data by about 10 - 30 ppb. Although there are very few aircraft observations above 1000 m AGL, what observations there are at this height indicate a pool of elevated ozone concentrations aloft. In addition, the aircraft data indicate that ozone should be <u>increasing</u> with height, whereas the ROM2.2/McIdas calculations <u>decrease</u> with height; the ROM2.2/McIdas layer 3 estimates at 1700-1800 m AGL are almost uniformly 42 ppb, whereas the observations suggest that ozone at this height should be twice as high.

Along the western boundary leg of the LMOS aircraft flight path on the morning of June 26 the ROM2.2/McIdas estimates are systematically less than the observed ozone in the southern half (41 - 42 latitude) by 15-55 ppb; the underprediction problem is smaller (7-30 ppb) on the northern section (42 - 43 latitude) of the flight. The western leg of the flight had more measurements above 1000 m AGL and confirm the presence of a large reservoir of elevated ozone (in excess of 100 ppb) above this height. ROM/McIdas ozone estimates at 1700 - 1800 m AGL (layer 3) along this western leg range from 42-55 ppb; the measured ozone values are in the range of 70-80 ppb.

In summary, the LMOS aircraft observations indicate that on June 26, 1991 the ROM2.2/McIdas simulation for LMOS episode 1 (June 22-29, 1991) significantly underestimates the amount of ozone being transported into the Lake Michigan region. This underprediction is especially severe on the morning of June 26 (the crucial time period for inflow of pollutants that will participate

in that day's ozone exceedances in the Lake Michigan region), when ROM underestimates the observed ozone above the surface layer by 10 - 55 ppb along the southern boundary, the most important inflow boundary. This systematic underprediction of the upper-level observed ozone concentrations entering the Lake Michigan region through the southern boundary persists throughout the day, although it is not quite as severe in the afternoon flights.

Several sensitivity tests are planned to assess the importance of this underestimation of the ozone boundary concentration for model results. A simulation using ROM results from layers 1 and 2 will be made; layer 3 will be excluded because concentrations are systematically lower than in the other layers. A simulation with boundary ozone concentrations scaled up by a linear factor will be made. In addition, a simulation will be made with modified boundary conditions prepared with ozone concentrations based on the observed data.

CONCLUSIONS

The LMOS photochemical modeling system consists of integrated components of current state-of-science meteorological, emissions, and photochemical grid models. The modeling system is currently being used to simulate an ozone episode that occurred June 24-28, 1991. In preliminary applications the model is predicting many of the important features of ozone formation in the Lake Michigan region, including the gradient in ozone concentrations along the lake shore. However, it is also underpredicting ozone peaks. One potential source of the underprediction is underestimation of the ozone boundary concentration, which is currently being investigated.

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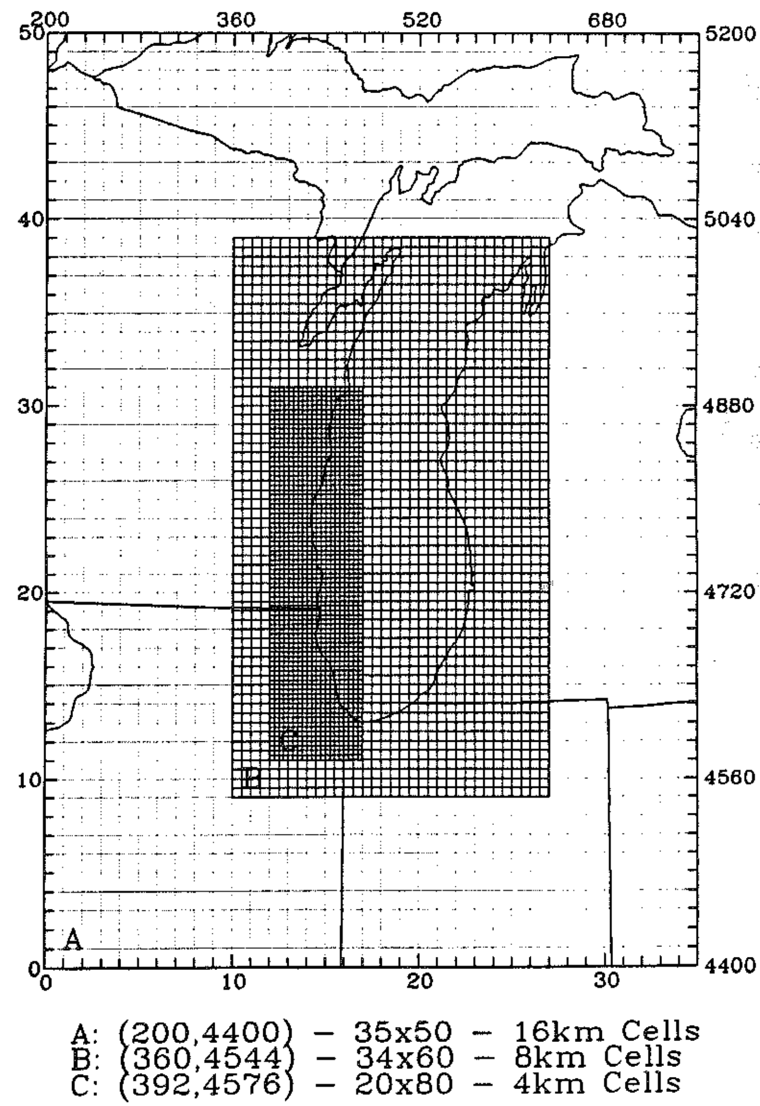

FIGURE 1. Nested-grid structure used in the application of the UAM-V to the Lake Michigan region.

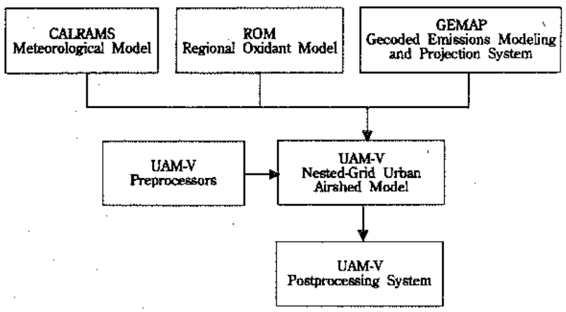

FIGURE 2. Structure of the LMOS photochemical modeling system.

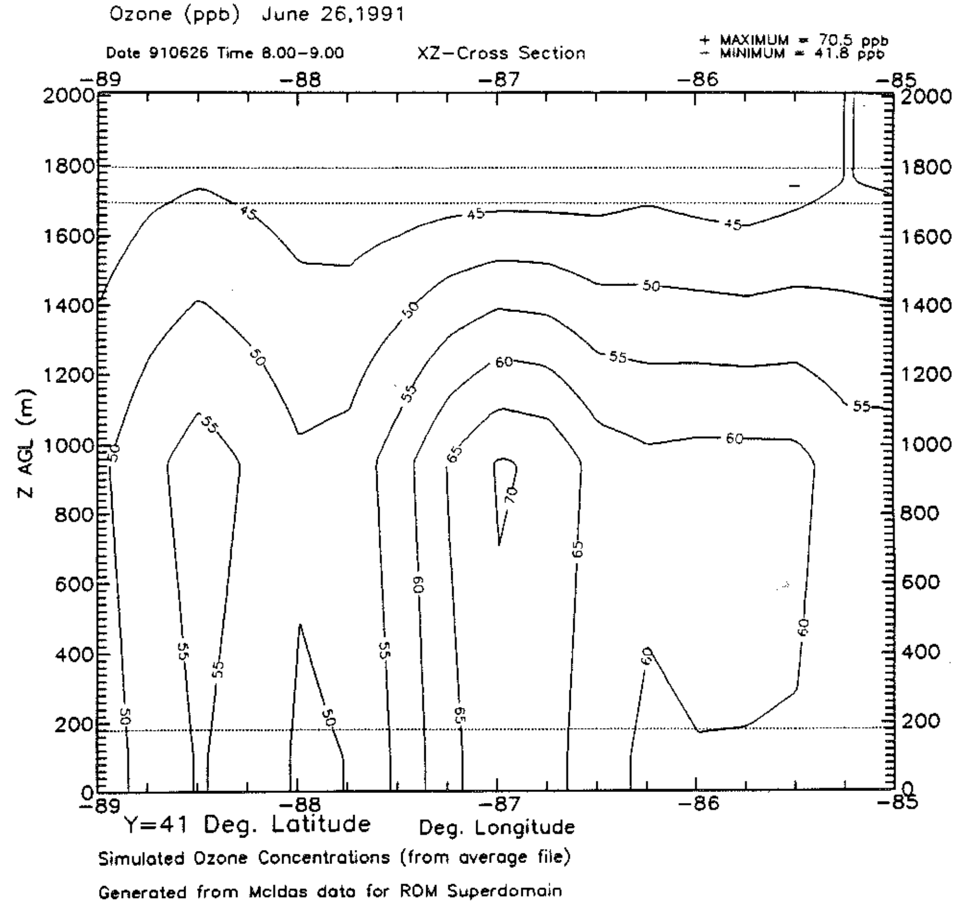

Figure 3a. ROM2.2/McIdas estimated hourly ozone concentrations (ppb) along the LMOS southern boundary flight path for the LMOS BOUNDARY aircraft morning flight on June 26, 1991.

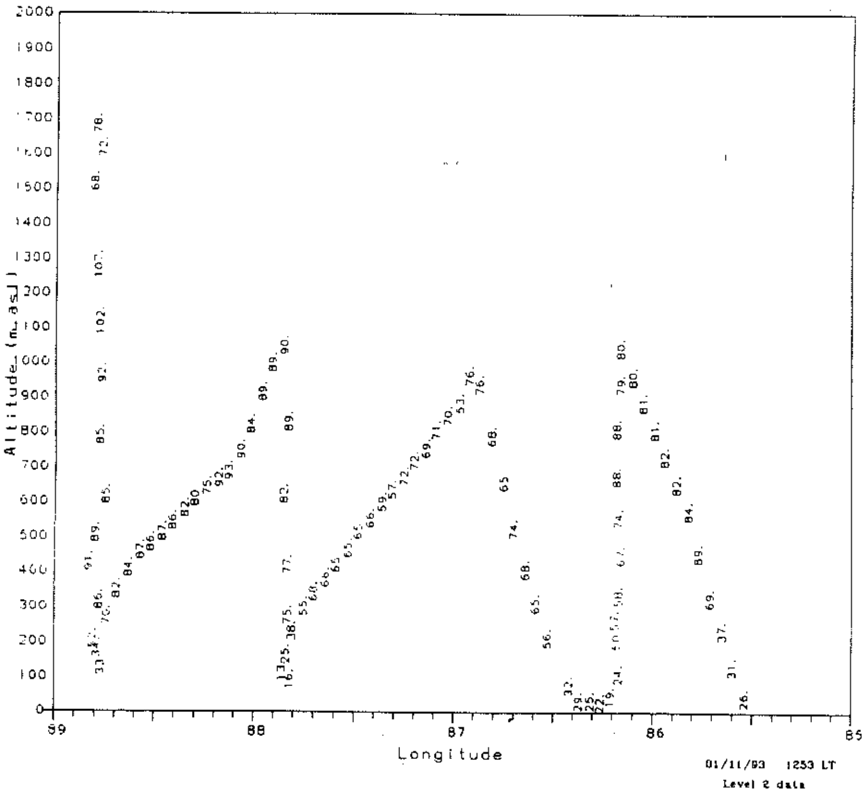

Figure 3b. Observed hourly ozone concentrations (ppb) along the LMOS southern boundary flight path for the LMOS BOUNDARY aircraft morning flight on June 26, 1991.

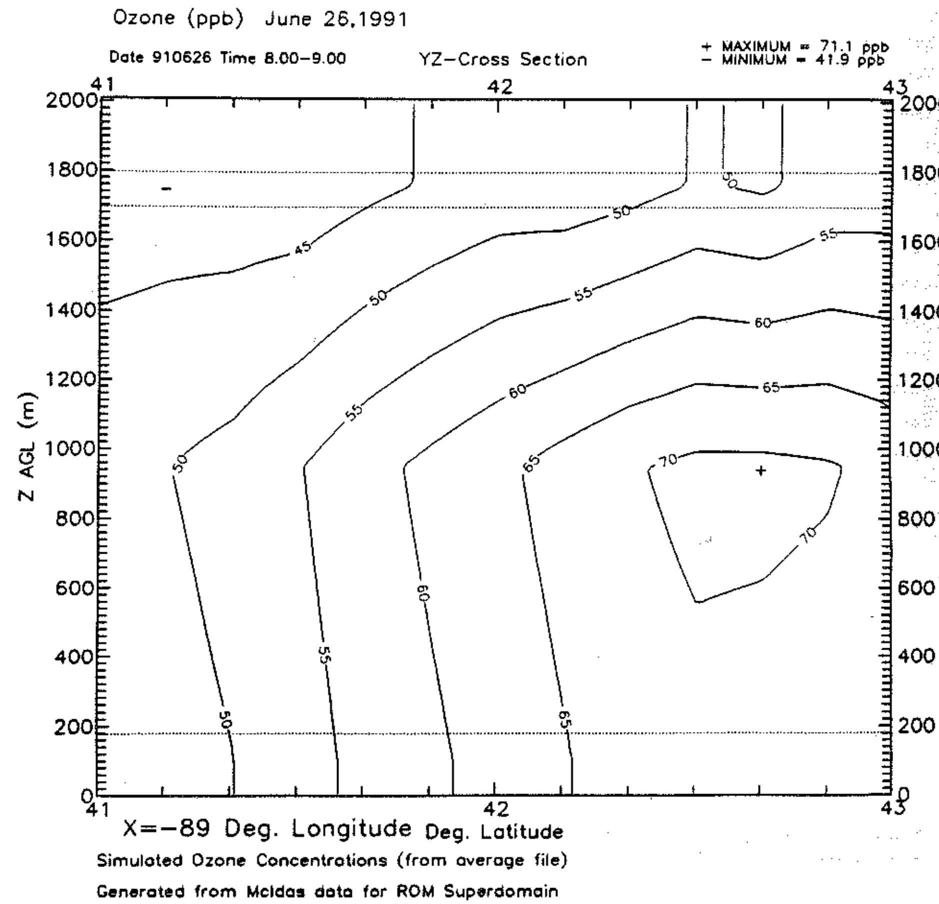

Figure 4a. ROM2.2/McIdas estimated hourly ozone concentrations (ppb) along the LMOS western boundary flight path for the LMOS BOUNDARY aircraft morning flight on June 26, 1991.

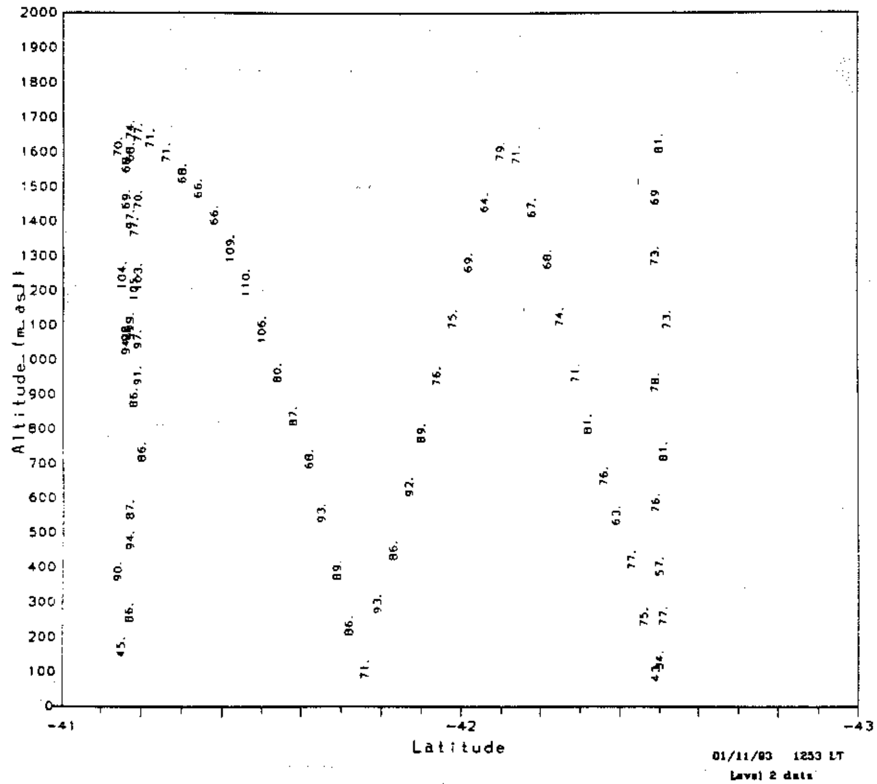

Figure 4b. Observed hourly ozone concentrations (ppb) along the LMOS western boundary flight path for the LMOS BOUNDARY aircraft morning flight on June 26, 1991.

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