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Project Summary

EPA Regional Oxidant Model: ROM1 Evaluation for 3-4 August 1979

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The first generation U.S. Environmental Protection Agency Regional Oxidant Model (ROM1) was tested and evaluated for O_3 predictions on a two-day test case episode in the northeast U.S. during 3-4 August 1979. The period was characterized by relatively high O_3 concentrations in the southern Great Lakes area where clear skies prevailed. The highest observed hour-average O_3 level monitored at a surface site during the period was 159 ppb. The ROM1 incorporates more simplifying assumptions and algorithms than the second generation version, ROM2, which is now in preliminary testing stages and will eventually become the production version of the model. Evaluation results for this test episode showed that the ROM1 had approximately a 6% average underprediction of O_3 when all hours and surface monitoring sites were considered. When the data were restricted to only those observed and predicted pairs of O_3 values greater than 50 ppb the average performance of ROM1 improved to a 1% underprediction. The evaluation phase concerned with estimating maximum daily O_3 values showed an 8% average underprediction of the maximum value for the restricted data subset. An analysis of individual O_3 plumes during the episode showed that the average model performance for predicting the plume maximum concentration level ranged from 22% underprediction to 38% overprediction.

The Project Summary was developed by EPA's Atmospheric Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The United States Environmental Protection Agency's Regional Oxidant Model (ROM) has been under development and testing for a number of years. The ROM attempts to simulate all of the important physical and chemical processes that affect the generation and dispersion of photochemical smog on regional scales (up to 1000 km). In the present configuration of the ROM domain, the model's horizontal resolution is approximately 18.5 km. In the vertical there are three and one-half layers. The first and second layers encompass most of the planetary boundary layer above the surface of the earth, and the third layer is the cloud layer extending from cloud base to near the tops of any cumulus-type clouds. Layer 0 is a shallow layer adjacent to the surface designed to treat sub-grid scale effects in the ROM. It is handled in a diagnostic manner within the model.

The model domain used in the first ROM application in the Northeast U.S. includes areas covered by special field monitoring projects during the summers of 1979 and 1980. During these projects highly resolved air quality, meteorological, and source emissions data bases were developed for the study area, hereafter referred to as the NEROS region (Northeast Regional Oxidant Study). The extent of the ROM1 domain in the NEROS application is 60 cells in the East-West direction and 42 cells in the North-South direction. The dimen-

sions of each individual grid cell are 15 minutes longitude (E-W) and 10 minutes latitude (N-S), or about 18.5 km^2 cells. The specific episode studied here occurred during 3-4 August 1979, during the first NEROS field project.

The ROM version used in this modeling study was the first generation model (ROM1). Several aspects of the ROM1 modeling system are in preliminary form as compared to the planned production version of the model, the second generation ROM2. One major difference between ROM1 and ROM2 is in the chemical kinetic mechanism. ROM1 contains a 23-species, 36-reaction-step mechanism developed by Dr. Ken Demerjian of EPA, whereas ROM2 will contain a 28-species, 70-reaction-step mechanism, Carbon Bond IV (CB-IV), developed by Dr. Gary Whitten of Systems Applications, Inc. The CB-IV mechanism contains an explicit reaction pathway for isoprene, a biogenic hydrocarbon species. This will allow the ROM2 to accommodate biogenic species in the source emissions inventory; ROM1 has no provision for biogenic species.

The data base used here to test and evaluate the 0_3 simulation results from ROM1 represents that of 3-4 August 1979. An assessment of the meteorological aspects of the data base indicated that the impact of the synoptic meteorological features on the photochemical smog potential over the NEROS study area were at a maximum from the Ohio Valley through the Great Lakes into Ontario for this two-day period. Wind speeds were light but of persistent direction in this area, and skies were clear. The eastern seaboard cities were under partially clear or overcast skies during the period. Surface wind directions were quite variable in the East also. The effects of these meteorological conditions were probably to suppress the photochemical potential in the East, although for brief periods during the daytime when skies cleared there would be a local increase in the potential.

The 3-4 August 1979 period was not a major episode for 0_3, although values exceeded 100 ppb in selected areas. On 3 August, despite the cloud cover over the mid-Atlantic seaboard, some 0_3 values reached between 100 and 115 ppb in the Washington and Philadelphia areas and between 120 and 130 ppb in the New Jersey, New York, and Connecticut area, where there was less cloud cover on that day. Measured 0_3 values of approximately 100 ppb were found downwind of Detroit and Toronto. Other measured values in the vicinity of the Great Lakes and Ohio Valley were not high, except near the southeast shore of Lake Erie, where Conneaut, Ohio recorded 159 ppb as the daily maximum.

On 4 August, the overcast and rainy conditions along the Atlantic coast from New York northward did, in fact, seem to suppress 0_3 generation. South of New York, however, relatively high levels were measured near the Philadelphia area (143 ppb) and Washington, D.C. (139 ppb) where skies had cleared. Several observation stations along the south shore of Lake Erie reported maximum 0_3 levels from 120 to 135 ppb. Most other areas of the NEROS region reported low values, except for a few observations near 100 ppb downwind of Detroit and Toronto.

Numerous aircraft transects were made over the NEROS region during the 3-4 August period. The temporal progression of flights from west to east reflects the Lagrangian sampling strategy of attempting to follow an area of high pollutant concentrations over the Midwest as it is transported east. Flights outside of the Lagrangian sampling were made as well. The aircraft data showed evidence of an area of elevated 0_3 concentrations aloft in the boundary layer to the south and east of the Lake Erie shoreline and possibly over the lake itself on 3 August. The timing and location of this area of high 0_3 concentration indicated that it was not generated on 3 August, but instead advected to the area from another time and location, quite possibly from Detroit and the heavy industrialized areas to the west of Lake Erie. A second 0_3 plume of urban-scale, probably from Detroit, was seen over western Ontario on 4 August. In general, the aircraft sampling during this two-day episode over the NEROS region indicated widespread boundary layer 0_3 levels of 70 to 80 ppb with some areas slightly higher or lower than this range at times.

Results

The ROM1 model was run for the 48-h period of 3-4 August 1979 using data from the NEROS and SAROAD data bases. The model was initialized throughout its entire domain with a set of tropospheric background species concentrations that were computationally adjusted for chemical equilibrium. The same set of concentrations was used for both lateral inflow and top boundary concentrations throughout the model simulation period.

The evaluation of the ROM1 results for 0_3 prediction was completed in several stages. First we compared model predictions, interpolated to the surface SAROAD station locations, with observed values over all hours and receptor sites. Next, an analysis of the maximum concentrations at receptor locations was made, and finally a thorough examination of individual plumes from large source areas within the domain was performed. We ignored the first 6 hours of predictions from the model because of the strong influence of initial conditions during this period.

The analysis of surface 0_3 observations and model predictions over all receptor sites and all hours showed that the diurnal range in 0_3 concentrations was considerably greater for the observations than for the model predictions, where an average variation of only 10 to 15 ppb was shown. Bias values, or observed minus predicted concentration values, were generally negative at night and positive during the day. The absolute values of bias (gross error) were all consistently rather high, indicating that the hours with average bias near zero actually contained a wide variation of individual values with opposite signs. The average episodic value of observed 0_3 for all hours at the surface monitoring sites was 38.9 ppb, and the corresponding model predictions for ROM1 layers 0 and 1 were 36.6 and 38.1 ppb, respectively. These values represent a 5.9% underprediction for layer 0 and a 2.1% underprediction for layer 1. Since these average 0_3 levels are near tropospheric background values, the significance of this analysis over all hourly values in the simulation period was not particularly great.

The next step in the evaluation was to perform an hourly analysis with a subset of the data values already used. The criterion for choosing the subset was based, in part, on the tropospheric background value of approximately 40 ppb 0_3 used in the ROM1's initial and boundary conditions and the fact that many of the surface monitoring site locations showed 0_3 predictions near this value. Therefore, the data subset was based on only those receptor points for which the observed value and the level 0 and 1 predicted values of 0_3 were

greater than 50 ppb. This should limit the data to those sites most affected by source emissions within the NEROS region. In fact, after this criterion was applied the number of sites used in the analysis dropped from near 150 during the midday hours to around 30, and from around 120 during the nighttime hours to 0.

The analysis of the data subset showed that the average observed concentration at the receptor locations varied from 51.0 ppb at 2000 h to 78.0 ppb at 1300 h on 3 August, and from 50.0 ppb at 0400 h and 0800 h to 80.7 ppb at 1600 h on 4 August. The corresponding predictions for layer 0 ranged from 56.0 ppb at 1900 h to 70.4 ppb at 1600 h on 3 August, and from 54.4 ppb at 0400 h to 76.2 ppb at 2000 h on 4 August. The average episodic value of observed O_3 in the data subset for all hours was 72.2 ppb, and the corresponding ROM1 predictions for layers 0 and 1 were 68.9 and 71.2 ppb, respectively. This represents an average O_3 underprediction of 4.6% for ROM1 layer 0 and 1.4% for layer 1, a slightly smaller degree of underprediction than the values computed for the full data set. The average values in the data subset were however, significantly greater than the tropospheric background O_3 value.

The most significant parameter of interest for the air quality policymaker concerning ambient O_3 is the daily hourly average maximum value observed at a monitoring station. The model evaluation for maximum O_3 concentration took place in two steps. First, in the local maxima analysis, model predictions of maximum hourly average O_3 levels at surface monitoring site locations were compared with measured values at the sites. Second, in the global maxima analysis, the concentration magnitudes and position of plumes of O_3 within the NEROS region were compared between the ROM1 predictions and the observations at surface monitoring sites, to the extent that these sites can define such plumes.

The local daily maximum O_3 concentration, c(max,ob), at a measuring site can be compared with the corresponding model prediction in two ways. First, the predicted maximum at the site, c(max,p0) for ROM1 layer 0 or c(max,p1) for ROM1 layer 1, can be compared to c(max,ob). Second, a more restrictive measure matches the prediction that occurs at the same hour as the observed maximum with the observed concentration [c(p0,h-ob) vs. c(max,ob) and c(p1,h-ob) vs. c(max,ob)].

A summary of average concentration data from the local maximum values analysis for the model simulation is presented in Table 1. Results from the full data set, as well as the data subset where all O_3 concentrations are greater than 50 ppb, are given. The number of receptor stations dropped from 156 in the full data set to 47 in the data subset. Interestingly, the average observed maximum value increased by only 2 to 4 ppb from the data set to the subset because there were very few observed maxima less than 50 ppb at the monitoring site locations. Conversely, the average model predictions increased by 20 to 30 ppb from the data set to the subset because of the large number of values near the background O_3 level. For the looser pairing of observed and predicted maximum values, the average bias at all receptor sites was 24.8 ppb on 3 August, representing a 34% underprediction and 25.3 ppb on 4 August, representing a 33% underprediction for model layer 0. For layer 1, the corresponding values were 23.2 ppb (32% underprediction) on 3 August, and 23.3 ppb (30% underprediction) on 4 August. In the data subset where the lower O_3 values are excluded, the results show a marked improvement. On 3 August, the average bias for layer 0 was 11.3 ppb (15% underprediction) and on 4 August, it was 5.6 ppb (7% underprediction). For layer 1 the corresponding values were 9.2 ppb (12% underprediction) on 3 August, and 2.7 ppb (3% underprediction) on 4 August.

The global maximum values analysis is performed to isolate for comparison individual areas or plumes of high O_3 concentrations from the model predictions and the ambient observations. The perspective of this analysis is broader than that of the local maximum values analysis in that model predictions at the same location as the observation are not necessarily required. Instead, the eligible area from which the model prediction is chosen is defined to be the coherent region of concentrations, or plume, from which the observation comes. This less restrictive pairing permits us to match observations and predictions based on supposedly similar phenomenological events in the physical processes producing the maximum O_3 values. This perspective also permits us to include a larger area than the single site location where the maximum value occurred.

In estimating model performance in terms of the global maximum perspective, we made three comparisons of model-predicted concentration with the maximum observed concentration, c(max,ob), in the O_3 plume. First, the maximum observed concentration was compared with the predicted maximum at the same location as the monitoring site of the observed maximum. Second, the observed maximum was compared with the predicted concentration at any of the monitoring site locations in or near the projected plume, and finally it was compared with the maximum concentration found in the grid cell at the center of the projected O_3 plume. These three values are designated (for ROM1 layer 1) as c(max,p1-A), c(max,p1-B), and c(max,p1-C), respectively. These comparisons range from the most restrictive to the least restrictive pairing of concentrations in the global maxima analysis.

Table 2 presents a summary of statistics from the global analysis of O_3 plume

*Table 1. Summary of ROM1 Results for Local Maximum O_3 Values for 3 - 4 August 1979**

	Full Data Set		Data Subset (all concentrations > 50 ppb)	
	79215	79216	79215	79216
Number of stations	156	154	47	48
Average c(max,ob)	73.2	77.8	75.5	81.8
Average c(max, p0)	48.4	52.5	64.2	76.2
Average c(p0,h-ob)	40.0	43.5	60.0	68.9
Average c(max,p1)	50.0	54.5	66.3	79.1
Average c(p1,h-ob)	41.6	45.1	62.0	71.4

*All concentrations are in ppb.

*Table 2. Summary of ROM1 Results for Global Maximum O_3 Values for 3 - 4 August 1979**

Urban Plume	Date	c(max,ob)	c(max,p1-A)	c(max,p1-B)	c(max,p1-C)
Detroit	3 Aug.	100	90	122	158
Toronto	3 Aug.	98	110	110	144
New York	3 Aug.	130	97	97	117
Detroit	4 Aug.	99	88	94	162
Toronto	4 Aug.	101	66	107	227
New York	4 Aug.	144	59	88	114
Philadelphia	4 Aug.	132	101	130	135
Average		115	87	107	151
S.D.		20	18	15	38

*All concentrations are in ppb.

maximum values. Seven individual plumes were considered. The average value of c(max,ob) recorded at surface monitoring sites in these plumes was 114.9 ppb. Three methods of pairing this observed value with ROM1 predictions were made. From the most restrictive to the least restrictive pairing the corresponding layer 1 model predictions averaged over the seven cases were c(max,p1-A) = 87.3 ppb, c(max,p1-B) = 106.9 ppb, and c(max,p1-C) = 151.0 ppb. The last predicted value is not restricted to measurement site locations, but can be at any grid cell within the predicted plume area. This measure has the greatest potential for overprediction, and in fact we would expect this to be the case because the density of measurement networks is rarely sufficient to capture the true O_3 peak value. The average bias for this pairing was −36.1 ppb, implying an average overprediction of about 31%. Note that if we drop from consideration the Toronto plume on 4 August, the average overprediction changes to about 23%. The very high predicted value over Lake Ontario, which could not be verified since the area was out of the range of the surface monitors, lends some support for this action.

The average bias in the most restrictive pairing for which the model prediction is interpolated to the same location as the monitoring station was 27.6 ppb, and the corresponding degree of underprediction was 21.6%. For the second comparison, where the maximum model prediction was restricted to monitoring site locations in or near the O_3 plume, but not necessarily at the site of the observed maximum, the average bias was 8.0 ppb with a corresponding degree of underprediction of 4.4%.

The variance in the values of overprediction or underprediction among the seven plume cases considered was indicated by the standard deviation (s.d.) about the average. For the two most restrictive pairings, the s.d. was approximately the same in each case, 21 to 22%. For the least restrictive pairing, the s.d. was approximately 54%, although much of that variance is attributable to the 4 August Toronto plume case. Although layer 0 predicted values were not considered in the global maximum values analysis, the results would not have been very different from those shown for layer 1. The layer 0 predicted maximum values were typically only a few ppb less than the corresponding layer 1 values.

Conclusions

The first generation Environmental Protection Agency Regional Oxidant Model (ROM1) has been evaluated for O_3 concentrations using the NEROS data base for the two-day test period, 3-4 August 1979. The evaluation proceeded in two stages. First, an overall analysis of O_3 observations and predictions at receptor monitoring locations in the model domain was made for all hours of the simulation except the first six. In the stage where all data were involved, results showed that, on the average, the ROM1 underpredicted O_3 levels by 6% in comparison with measurements at monitoring sites. In a second part of the first stage of analysis, the same manner of evaluation was applied to a subset of the data where only simultaneous O_3 values above 50 ppb were included for observed and predicted concentrations at monitoring sites. In this case, the average ROM1 performance for the data subset showed a 4.6% underprediction for layer 0 and a 1.4% underprediction for layer 1.

The second aspect of model evaluation, using daily O_3 maxima, also proceeded in two steps. In the first step, the daily maximum value at each receptor location was compared to the predicted maximum at that location as well as the prediction made for the same time as the observed maximum. For layer 1, the ROM1 performance showed an average 31% underprediction for the first comparison and a 43% underprediction for the second comparison. Results for layer 0 were similar. When data were restricted to those observed and predicted O_3 pairs above 50 ppb, the model performance for the local maximum analysis improved by showing average underpredictions of 8% and 15%, respectively, for the above layer 1 comparisons. The improvement in model predictions in this case was primarily due to restricting the analysis to comparisons at monitoring stations locations where source emissions had a larger effect on O_3 levels than material that was present initially and was overlooked by the clean initialization procedure.

The second step of evaluating the ROM1's performance for O_3 maxima predictions involved an analysis of individual plumes of O_3 from major source areas within the NEROS region. Seven cases of such plumes were identified and analyzed for the 3-4 August 1979 episode. The evaluation used three types of comparisons of O_3 maxima ranging from a strict spatial pairing between observed and predicted values to a fairly loose spatial pairing. Results averaged over the seven plumes in the test case showed a 22% underprediction for the strictest paired comparison, a 4% underprediction for the intermediate comparison, and a 38% overprediction for the loosely paired comparison. The uncertainty of these aspects leads one to conclude that the results presented here are probably bounds on the actual model performance. The ROM1 tended to perform better in those areas of the domain where a well-organized flow field was present and the assumption of clean initial conditions was not grossly violated. Applications with the

second generation regional model, ROM2, should be able to quantify the model performance to a greater degree than was done in this case.

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The complete report, entitled "EPA Regional Oxidant Model: ROM1 Evaluation for 3-4 August 1979," (Order No. PB 86-215 886/AS; Cost: $16.95, subject to change) will be available only from:

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