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Project Summary

Evaluation of the Regional Oxidant Model (Version 2.1) Using Ambient and Diagnostic Simulations

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This Project Summary discusses an evaluation of the latest version of EPA's Regional Oxidant Model, ROM2.1. In the ambient evaluation, model estimates were compared with ambient measurements of hourly surface ozone collected on 26 days during the summer of 1985 in the northeastern United States. Observed and modeled maximum daytime concentrations agreed, on average, to within 2 ppb (79 ppb versus 77 ppb). The model tended to underestimate at the higher extremes of the frequency distribution. The 95th-percentile value was underestimated by 8 ppb (127 ppb versus 119 ppb). Underestimates at the upper percentiles were more prevalent in the southern and western portions of the model domain. Estimated and observed spatial patterns of three day maximum ozone generally showed good agreement. ROM2.1 improved noticeably over ROM2.0 with regard to the orientation of the high-ozone plumes in the Northeast Corridor. A unique aspect of the ambient evaluation was an assessment of the model's ability to estimate boundary conditions for the Urban Airshed Model. Near New York City, estimated and observed boundary conditions agreed to within 4 ppb (57 ppb versus 61 ppb). Model performance was degraded, however, during some situations with dynamic mesoscale wind flow conditions. ROM2.1 also underwent a series of diagnostic tests to investigate the accuracy of its numerical solution algorithms. When the model was subjected to extremely steep concentration gradients (steeper than those observed in the ambient atmosphere), the model did not conserve mass during a 48 h simulation, deviating by as much as 18% from the initialized value. However, tests with a mass-corrected version of the full simulation model showed that predicted ozone values deviated only slightly (less than 4%) from the original model.

This Project Summary was developed by EPA's Atmospheric Research and Exposure Assessment 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

After realizing that summertime episodes of photochemical smog were a regional and not a localized urban phenomenon, EPA embarked on a research program in the middle 1970s to develop a regional-scale computer model for simulating the transport and fate of ozone (O_3) and its precursors. In 1983, this work resulted in the first operational version of the EPA Regional Oxidant Model (ROM1). Testing of ROM1 and analysis of field data prompted additional improvements, including the ability to model biogenic emissions, horizontally-varying layer thicknesses, and improved deposition relationships. After a period of development, the first application version

of the ROM (Version 2.0) was completed in 1986. It has since been used for several studies in the Northeast and the Gulf Coast regions of the U.S., and it has undergone an intensive evaluation using field data collected in 1980.

Additional needs by the northeastern states and the emergence of new model improvements prompted the development of ROM2.1. Improvements to ROM2.1 over ROM2.0 included an expanded modeling domain, an updated methodology for computing biogenic emissions of hydrocarbons, revisions in the objective wind field interpolator to remove known biases in the low-level wind flow, and a more sophisticated anthropogenic emissions processor.

Creation of ROM2.1 was primarily motivated by the Regional Ozone Modeling for Northeast Transport (ROMNET) project. In general, the objective of ROMNET is to investigate interurban transport of ozone and its precursor emissions in the Northeast U.S. to support state air pollution control agencies in the development of State Implementation Plans to achieve the National Ambient Air Quality Standard (NAAQS) for O_3. In this regard, ROM is being used to estimate regional O_3 concentrations and to examine the effectiveness of a variety of hydrocarbon (VOC) and nitrogen oxides (NO_x) emissions control strategies for reducing O_3. Another major objective of the ROMNET project is to use ROM calculations for deriving boundary conditions for urban-scale applications with the Urban Airshed Model (UAM). Because of ROM's importance for comparing the estimated effectiveness of emission control strategies and for estimating boundary conditions, representatives of the ROMNET project asked EPA's Office of Research and Development to evaluate the performance of ROM2.1.

The approach we took complements the evaluation of ROM, Version 2.0. The primary difference between the two evaluations is that the ROM2.0 evaluation used a special field-study data set from 1980, while our evaluation used routinely-collected data from 1985. Our evaluation, unfortunately, could not be as comprehensive as the ROM2.0 evaluation, which had access to extensive field measurement data for ozone, hydrocarbons, and nitrogen oxides as well as aircraft transects. We were able to use only routine data stored in EPA's Aerometric and Information Retrieval System (AIRS). Therefore, the ambient evaluation of ROM2.1 was limited to hourly observations of surface ozone from state and local agency monitoring sites.

In this project, we compared observed and modeled ozone concentrations for selected periods of high ozone observed during the summer of 1985. Periods from 1985 were chosen because they correspond to the base year emissions inventory. The objectives of the ambient evaluation were (1) to examine overall evaluation statistics to determine whether a general bias exists in the model calculations, (2) to look at spatial patterns of maximum concentration to determine whether a spatial bias exists, and (3) to examine the model's applicability for determining UAM boundary conditions.

In addition to the ambient evaluation, we performed a series of "stressful" diagnostic tests on the model. In the original development of the first generation ROM (ROM1), a number of diagnostic tests were performed to probe the accuracy of the numerical algorithms used to solve the equations that simulated physical and chemical processes. These tests were designed in a hierarchial fashion beginning with a chemistry-only simulation. Transport was added to the chemical simulation, then vertical mixing, and finally source emissions. These tests represented the next step after independent (external to the ROM framework) tests of the model's numerical algorithms. Results from this original set of diagnostic tests demonstrated that the model faithfully represented solutions to the relevant equations.

Since the time of ROM1, numerous changes have been made to the entire ROM modeling system culminating in the most recent version of the second-generation ROM model (ROM2.1). Although there were significant changes to the chemical and physical processes simulated within the ROM, few changes were made to the basic numerical algorithms employed to solve these processes. Nevertheless, a new round of diagnostic testing was proposed for ROM2.1 that would complement the earlier work done with ROM1. We performed these diagnostic tests on the production version of ROM2.1 used for the ambient evaluation. In the diagnostic evaluation, the accuracy of the numerical algorithms was assessed by evaluating the model's ability to conserve mass for these diagnostic tests.

Ambient Evaluation

Because we wanted the model simulations to correspond to the base year of the 1985 NAPAP emissions inventory, we examined ozone monitoring data from 1985 for candidate episodes. In particular, we were interested in periods when ozone exceedances (hourly concentrations greater than 120 ppb) were observed throughout the Northeast Corridor. After identifying two candidate episodes, we examined these episodes further for possible starting and ending dates for model simulations, recognizing that the ROM is designed for three-day segments starting at noon and that the first segment should be initialized with "clean" (low ozone/precursor concentrations) conditions. The episodes selected for modeling were July 7-22 and August 7-16.

Two types of databases were assembled for the ambient evaluation: hourly concentrations of ozone from (1) model estimates and (2) observations. To produce the modeled database, we executed the ROM for the two episodes. Model inputs included National Weather Service surface and upper-air meteorological data, observed ozone concentrations for estimating boundary conditions, and hydrocarbon and nitrogen oxide emissions (both anthropogenic and biogenic).

The ROM is a three-layer Eulerian grid-scale model that estimates hourly photochemical species concentrations for a 64 by 52 grid. Each grid cell is 1/6° latitude by 1/4° longitude, or approximately 19 km by 19 km. For this study, we evaluated only hourly ozone concentrations from layer 1, because concentrations from this layer most closely represent surface ozone observations. In layer 1, an individual grid cell is typically ~100 m in vertical extent at night, and 200-500 m deep during the day.

We developed three different model databases for the evaluation. (1) Point estimates from gridded data: For the portion of the evaluation concerned with general statistics, we interpolated gridded estimated ozone values to actual monitoring locations using a biquintic interpolation scheme that is consistent with the method used in the model. (2) Contoured values of gridded data: For analyzing spatial patterns, we used an objective contouring algorithm to produce computer graphics depicting concentration fields based on the gridded ROM data. (3) Interpolated values derived using the ROM/UAM interface method: For the portion of the evaluation concerned with boundary conditions, we employed a fairly elaborate interpolation scheme, described in the project report, that is consistent with the ROM/UAM interface developed for the ROMNET

program. This interpolation allowed us to transform boundary conditions from ROM's 19-km grid size to the grid size of the UAM domain, typically 4 to 10 km.

Analogous to the model databases, we developed three observation databases: (1) a set of observations used for developing overall statistics; (2) a set of observations used for creating contour plots; and (3) a set of observations used for developing UAM boundary conditions. We obtained ozone concentrations from monitoring data archived in EPA's Aerometric Information and Retrieval System (AIRS), which contains a national database of hourly ozone (O_3) concentrations and information on monitoring sites. Hourly O_3 concentrations were selected for sites located in the U.S. portion of the ROMNET domain for the two episodes that we modeled with ROM. (Canadian O_3 monitoring data are not included on AIRS and were not readily available for this analysis.) An extensive review and screening of the data was performed. We included only daytime values (0800 h LST to 1900 h LST) in the evaluation because nighttime observations are influenced by localized processes that often include scavenging of O_3 by NO_x emissions and therefore do not reflect vertically-integrated O_3 concentrations in layer 1 of the ROM. Furthermore, we excluded a site's data on days missing more than 25% of their observations. We also examined the data for extremely high or low values. Several sites, such as Poughkeepsie (NY), were eliminated because mean daytime O_3 concentrations were consistently below 50 ppb and may have reflected local NO_x scavenging. Of the more than 200 sites in the original database, 187 of these were used in computing general statistics. For portions of the analysis, the data were divided into five geographical groups.

The monitoring data used for developing the UAM boundary condition database were given special consideration. The approach we followed is consistent with previous modeling studies that used monitoring data to prescribe UAM boundary conditions. The assignment of sites to a boundary location depended on the prevailing wind direction for that day. If more than one site was available for a location, the hourly concentrations were averaged. After averaging at six locations along the UAM boundary, concentrations were spatially interpolated (using linear avearaging). To be consistent with the ROM/UAM interface method, we then used the hourly concentrations to create three-hour running averages.

In the ambient evaluation portion of the study, we found good overall agreement. For a 26 day simulation, mean concentrations of the modeled and observed daily maximum concentrations agreed to within 1%. Concentrations at the higher ends of the frequency distributions were slightly underestimated; the 95th-percentile observed daily maximum concentration was 127 ppb while the estimated concentration was 119 ppb. The tendency to underestimate peak concentrations is to be expected with a coarse grid model such as the ROM because of the spatial averaging that occurs with Eulerian grid computations.

In the Northern Corridor and Southern Corridor geographical groups (groups 1 and 2, respectively), model performance was good, particularly in group 2. The group 1 mean observed and modeled daily maxima agreed to within 11% and the 95th-percentile observed and modeled daily maxima agreed to within 5% (both values were overestimated). For group 2, the mean daily maxima were within 3% of each other and the 95th-percentile values were within 7% (both values were underestimated). The quantile-quantile plots of observed and modeled daytime hourly concentrations showed the same kinds of tendencies: overestimation in the upper quantiles of group 1 and underestimation in the upper quantiles of group 2, as well as better overall agreement for group 2 than for group 1 – only the top 15% of group 1's estimates were within 10% of the observations, while for group 2 the top 70% of the estimates were within 10% of the observations. The medians in the time series plots of daily maxima for these two groups showed analagous underestimate-overestimate tendencies, and these plots also showed that exceedances (values over 120 ppb) were overestimated in group 1 (ten versus eight) and underestimated in group 2 (six versus ten).

Model performance in group 3 (the southwestern part of the domain – southern Virginia, West Virginia, Ohio, and western Pennsylvania), an area removed from the extensive metropolitan area of the Northeast Corridor, was noticeably poorer than the performance for groups 1 and 2. The group 3 mean daily maximum was underestimated by 12% and the 95th-percentile daily maximum was underestimated by 19%. The quantile-quantile plot for group 3 showed that the top 35% of the values were underestimated by more than 10%. The group 3 time series plot showed that 12 out of 14 medians were underestimated, and that exceedances were dramatically underestimated (six versus zero). Underestimates of upper-quantile concentrations in this group perhaps can be attributed to the relatively small-scale urban plumes and uncertainties in estimating naturally-occurring emissions of NO_x and hydrocarbons. However, deficiencies in anthropogenic emissions inventories should not be ignored and ongoing efforts to improve them should continue.

Groups 4 and 5 (the northern part of the domain, excluding the Northeast Corridor) had observations close to background values, and model estimates generally showed good agreement with observations, especially for the upper values.

Spatial patterns of the three-day maximum concentrations usually showed reasonable model performance. The modeled magnitude and orientation of ozone plumes in the northern portion of the Northeast Corridor, especially around New York City, compared well with observed plumes. The model also did an excellent job of predicting high ozone levels around coastal sections of Maine. We believe that ROM2.1 performed better than ROM2.0 in these areas because ROM2.1 includes a correction for the westerly bias that occurred in ROM2.0's low-level wind flows. Differences between observed and modeled plumes were most evident during episodes experiencing coastal troughs and squall lines. Underestimates in the Washington, DC, area that were reported in the ROM2.0 evaluation were seen again in our evaluation. In addition, ROM 2.1 tended to underpredict rural peak concentrations of ozone by about 20 ppb. Few monitoring data are available for evaluating model performance in rural areas, so it is hoped that measurements being taken under the auspices of the National Acid Precipitation and Assessment Program (NAPAP) will aid in future evaluation of ozone concentrations.

The most rigorous portion of this analysis was an evaluation of the model's ability to estimate boundary conditions for UAM application. Although we do not recommend applying the ROM in a deterministic manner, some type of reliable estimation scheme is needed for prescribing boundary conditions when the UAM is to be applied for future-year emission control strategies. Also, model estimates are needed because measurements aloft are typically not available for specifying the vertical structure of pollutant concentrations. Furthermore, our

analysis showed that using monitoring data to estimate boundary conditions requires a great deal of subjectivity and is fraught with uncertainty.

Overall, ROM2.1 estimates compared quite well with the monitoring data for estimating UAM near-surface boundary conditions in the OMNYMAP domain. The model overestimated the mean concentration for all daytime hours by just 5 ppb (8%) and underestimated the 95th-percentile value by 9 ppb (9%). However, we saw significant day-to-day variability in model performance, ranging from a maximum underestimate of 24% to a maximum overestimate of 49%. A case study performed for July 10, 1985, demonstrated that small-scale meteorological features can cause dramatic effects on model performance, apparently because such features are not captured in the ROM's overall interpolation of meteorological data. We found that a squall line resulted in a significant overestimate in ozone concentrations along UAM's western boundary (the inflow boundary on that day). We therefore caution UAM users to carefully review ROM estimates and be aware of mesoscale flow conditions. On most days, however, ROM2.1 did a reasonable job estimating UAM boundary conditions.

Diagnostic Tests

In order to perform diagnostic tests on ROM2.1 and its most critical processors under known atmospheric conditions, a specialized processor system has been developed to allow the specification of certain wind field and model layer patterns in an analytically defined atmosphere. By predetermining the wind field and model layer depth patterns in time and three-dimensional space, the capacity of the ROM and specific processors to obey various physical laws may be tested.

Particular wind flow and layer definition sets for each test case are defined. Also defined are the wind field and the vertical layer boundaries, each of which may be dependent on the various physical quantities that are analytically set in an earlier meteorological processor. Eight diagnostic test cases are defined. Horizontal diffusion due to turbulent eddies is set to zero for these tests. The temperature lapse rate is defined to be adiabatic, which is a good approximation for the actual atmospheric mixed layer where the ROM is designed to work. The only atmospheric definitions which do not approximate the real atmosphere are the neglect of the effect of water vapor on the specific gas constant for air and the assumption of no horizontal diffusion due to turbulent motion. The neglect of water vapor effects is necessary to achieve a tractable solution of the atmospheric definition equations.

Test case 1A is designed to test the horizontal transport and interlayer mass flux mechanisms in the model. For this test case, a circular anticyclonic wind field is specified identically for all three model layers. A temporally oscillating pattern of ROM layer depths was used to provide the mechanism for vertical mass flux between ROM layers. The three layer tops are kept horizontally flat at all times, with the heights of the top of layer one and two oscillating up and down in time. The depth of the full model domain is fixed over all space and time (1500 m). For test case 1A, all chemical reactions are turned off in ROM2.1. Only one chemical species, used as a mass tracer, is given a spatially-dependent initial concentration that differs from the prescribed background concentration. This species is given a conical-shaped initial concentration distribution. It should be noted that the initial concentration magnitudes are completely arbitrary, because the chemical reactions are turned off for this test case.

Results of this test show an oscillation in the mass field over time. The periodicity corresponds to that of the oscillation in the ROM layer depths for this test. Mass increases as much as 6% in the model domain during the first third of the simulation. Later, a mass decrease of around 2% is evident. The overall trend in the mass field is toward a decrease over time. The degree of mass change is not strong here, although the test does suggest that mass conservation errors may occur when the model layer interfaces change significantly over time.

Test case 1B is very similar to 1A, except that the layer heights vary over space instead of over time. This case is also designed to test the transport and numerical algorithms of the model. The wind field and the initial concentration fields for the three ROM layers are the same for test 1B as they were for 1A. Results for test 1B show that the mass total remains within close proximity of the original mass amount during the simulation. Maximum changes of about 4% from the original mass are seen.

Test case 1C is designed to examine the accuracy of the numerical transport scheme alone, without vertical fluxes occurring. The wind field and initial mass fields for each ROM layer used here are identical to those used for test case 1A. The layer top heights are horizontally flat and are constant in time for test 1C. This allows for an examination of the ability of the ROM to conserve mass during periods of rotational (non-divergent) flow with no vertical transport across the layer interfaces. Results show that the total mass within the domain grows by nearly 7% in the first third of the simulation, and then stabilizes later at a mass increase of approximately 8% over the initial mass. Considering that there are no physical or chemical sources or sinks of mass in the model simulation, this is a significant mass increase.

Test case 2 is a somewhat more complex test of the numerical transport algorithms in the ROM. For this test case, a purely divergent (convergent) flow field is used. The layer average wind fields for each of the model layers are identical, resulting in no vertical wind shear. A west-to-east zonal wind field is defined for each layer such that speed maxima exist along the western and eastern boundaries of the modeled region, and speed minima exist along the central longitude of the modeled region.

It was desired for test case 2 that the layer boundaries represent material surfaces, or surfaces across which there is no flux of material. Thus, the layer heights must be determined such that, given the layer average wind fields and the analytically defined physical variables, there is no transport of air across the layer boundaries. This stipulation requires that the layer heights be determined based on the defined wind field.

Results show that during the first half of this simulation the total mass increases by nearly 18% within the grid. This corresponds to the region of convergent winds and increasingly deep layer heights. As the cloud mass enters the region of divergent winds and increasingly shallow layer heights the mass increases level off and eventually the mass begins to decrease. This decrease, however, occurs at a much slower rate than the earlier mass increase, thus resulting in a net mass increase of approximately 13% at the end of the simulation.

In test 0, we attempt to simplify the transport environment to isolate the cause of the mass increase. The ROM layer heights for test case 0 were spatially and temporally constant over the model domain and were set at the values used in test case 1C. The wind field prescribed was essentially constant in space and time. The initial concentration field for test 0 was similar to that specified for test case 1A.

Results for this test show a total mass increase of about 10% toward the end of this simulation. This result is significant because the test has isolated the numerical errors to the horizontal transport scheme, without the complicating effects of vertical redistribution of mass.

To determine the degree to which the noted mass increases from the numerical advection algorithms were a function of the magnitude of initial concentration gradients, a second test (test 0A) was performed in which the concentration gradient was diminished by nearly a factor of four.

Results from test 0B show that mass is essentially conserved during the simulation, with a mass increase of only 0.6% at the end of the simulation. The contrast between the results of this test and test 0 demonstrate that the numerical artifact of the mass increase is a function of the magnitude in concentration gradient.

In the final test case (0B) presented here, we investigate the effect of "clipping" negative concentration predictions from the model run. Small negative ripples of concentration near the edges of large concentration gradients are produced when these gradients are advected. The negative concentrations are a result of the limitations of finite difference approximations to large sub-grid gradients. The negative values, in themselves, do not pose a problem for the advection routines. However, when the advection solution is passed to the chemistry portion of an air quality model, there must be no negative concentrations since these are not defined in a chemical simulation. Negative values produced by ROM's numerical transport solution are "clipped", or set to 10^{-16}. Since we are not solving the chemical equations in these analytical tests, it is possible to retain any negative concentrations resulting from the transport simulation. In test case 0B we have suppressed the negative clipping and allow the propagation of any negative concentrations.

The layer depths are the same as those used in test case 0, constant in space and time. The wind field is also the same as in test case 0, simple zonal flow. The initial concentration field is the same as that used in test case 2. Results indicate an initial increase of mass of about 0.5%, dropping back to about 0.4% for the remainder of the simulation. This value should be compared to the nearly 10% (and rising) normalized mass ratio at the end of the test 0 simulation. It is apparent that the clipping of negative concentrations has introduced a significant mass increase during the advection of sharp concentration gradients.

To test the effect of "clipping" negatives in actual ambient ROM simulations, a two-day simulation was performed for July 6-7, 1988, a particularly severe ozone episode in the Northeast U.S. In addition to the base run, containing any mass imbalances caused by the "clipping" of negatives, a simulation was performed in which a first-order correction was made to the advected concentration field to assure mass conservation.

Results show that the differences between the corrected and uncorrected simulation results were almost always less than 1%. Differences seen in the NO_x concentrations were greater than those of the other species, but generally under 10%. These results suggest that the implementation of a mass-correcting scheme in ROM's numerical advection algorithm would be a desirable, although probably not essential feature. We plan to repeat the diagnostic tests discussed here with the global mass-correction algorithm in place and analyze the results in detail.

Summary and Recommendations

Using both an ambient evaluation and a series of diagnostic tests, we evaluated Version 2.1 of the Regional Oxidant Model (ROM2.1). In the ambient evaluation, we assessed ROM2.1's performance for periods of high ozone in July and August of 1985 in the northeastern U.S., using AIRS daytime hourly surface ozone monitoring data. We compared these observations with model estimates in three types of analyses: (1) a comparison of overall statistics to determine whether model estimates exhibited a general bias, (2) a comparison of spatial patterns of maximum concentrations to look for spatial bias in the model estimates, and (3) an assessment of the model's applicability for determining UAM boundary conditions. In the diagnostic tests, we assessed the accuracy of numerical algorithms by evaluating the model's ability to conserve mass; we performed five tests that involved only the horizontal transport algorithm and two that involved both horizontal transport and vertical flux.

In the ambient evaluation, model estimates were compared with ambient measurements of hourly surface ozone collected on 26 days during the summer of 1985 in the northeastern United States. Observed and modeled maximum daytime concentrations agreed, on average, to within 2 ppb or 1.4% (79 ppb versus 77 ppb). The model tended to underestimate at the higher extremes of the frequency distribution. The 95th-percentile value was underestimated by 8 ppb or 6.6% (127 ppb versus 119 ppb), and the overall maximum value was underestimated by 50 ppb or 22.7% (219 ppb versus 169 ppb). Underestimates at the upper percentiles were more prevalent in the southern and western portions of the model domain. Concentrations at the lower end of the frequency distribution were slightly overestimated. Estimated and observed spatial patterns of three day maximum ozone generally showed good agreement. ROM2.1 improved noticeably over ROM2.0 with regard to the orientation of the high-ozone plumes in the Northeast Corridor and the depiction of high concentrations along the coast of Maine. Similar to ROM2.0, a tendency to underestimate peak concentrations near Washington, DC was again evident with ROM2.1. A unique aspect of the ambient evaluation was an assessment of the model's ability to estimate boundary conditions for the Urban Airshed Model. Near the New York City metropolitan area, estimated and observed boundary conditions agreed to within 4 ppb or 7.6% (57 ppb versus 61 ppb). Model performance was degraded, however, during some situations with dynamic mesoscale wind flow conditions.

In the second part of our evaluation, we employed a series of diagnostic tests to assess the model's ability to conserve mass. For test cases 1A and 1B, in which mass flux was allowed between layers, mass changes were expected to occur in individual model layers. For the other tests, however, no change in mass was expected for individual layers. For all tests, there should have been no change in mass for all layers combined (total domain).

For most test cases, there were serious departures from mass conservation. Only in test case 0A (where the concentration gradients were considerably relaxed) and test case 0B (where negative clipping was suppressed) was the total domain mass effectively conserved. The results for the other five test cases suggest a potential problem with the ROM's numerical transport procedures, despite earlier design tests performed during the ROM's developmental stages that showed no problems with mass conservation. We have delayed further diagnostic tests, including examining test case 3 with chemical simulation, and further analysis, including preservation of peak concentrations, until

the mass conservation problem has been corrected.

A first-order correction algorithm has been developed based on a global assessment of the mass imbalance due to the clipping of negative concentrations. This algorithm was implemented and tested on a two-day ambient simulation during a high O_3 concentration period. Results have shown that the differences between the corrected and uncorrected simulation results were almost always less than 1%. Differences seen in the NO_x concentrations were greater than those of the other species, but generally under 10%. These results suggest that the implementation of a mass-correcting scheme in ROM's numerical advection algorithm would be a desirable, although probably not essential feature. We plan to perform further tests to assess the degradation in computation time with the inclusion of the mass correction scheme. With this additional information, we will weigh the improvements in accuracy of the transport solver with the increases in computation time. We will also repeat the diagnostic tests discussed in this section with the global mass-correction algorithm in place and analyze the results in detail. Our analysis has demonstrated the value of this type of diagnostic testing in model evaluation.

Our evaluation has suggested that further improvements to the ROM are warranted. We are improving the specification of layer thicknesses and the computation of naturally-occurring emissions. In future years, we hope that a dynamic meteorological processor can be incorporated that will simulate non-steady state flows. To continue making advances in model development, additional monitoring data are needed for examining other chemical species (such as NO_x, isoprene, formaldehyde, and HNO_3) and for fully evaluating model performance in rural areas.

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The complete report, entitled "Evaluation of the Regional Oxidant Model (Version 2.1) Using Ambient and Diagnostic Simulations," (Order No. PB 90-225 293/AS; Cost: $23.00, subject to change) will be available only from:

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