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A Review Of Recent Applications of The SAI Urban Airshed Model

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1. INTRODUCTION

The U.S. Environmental Protection Agency has sponsored a series of studies on the use of the SAI Urban Airshed Model in the development of strategies for ozone control in urban areas. Completed studies include those in Tulsa, Denver, and St. Louis. Additional work in Los Angeles has been sponsored largely by groups other than EPA. The four cities are similar to the extent that all are relatively isolated from the influence of other urban regions. However, their size and the amounts and types of data available for modeling vary widely. The purpose of this report is to summarize and compare the major findings of these studies so that future users of the model will know what to expect and know best how to use the resulting information.

The report is organized as follows. Section 2 gives a capsule description of the SAI Urban Airshed Model. Section 3 provides a brief synopsis of data bases and methods for each study. The remaining sections attempt to integrate the results of all the studies. Evaluation of model performance, a major focus of all four studies, is covered in Section 4. Section 5 examines model sensitivity, emphasizing selected results. Results of applying the model to control strategy assessment are discussed in Section 6. Summary remarks and overall perspectives regarding the model are presented in the final section.

2. DESCRIPTION OF THE MODEL

The SAI Urban Airshed Model simulates the major physical and chemical processes associated with ozone formation in the polluted troposphere. These include gas phase chemistry, advective transport, and turbulent diffusion. The modeling domain is divided into a large array of grid cells. Horizontally the cells are uniformly sized squares 3 to 5 kilometers on a side. Typically, four or five layers of cells represent the vertical domain. The depth of the layers is scaled by the height of the mixed layer and the height of the top of the modeling domain (region top). The latter typically ranges from 500 meters in the morning hours to 1000 meters or more in the afternoon. Emissions are injected into individual cells depending on the location of the sources, their height of release, and the buoyant rise of individual stack gas plumes.

The theoretical basis for the SAI Urban Airshed Model rests on the conservation of mass equation for atmospheric diffusion. Each reactive species is subject to chemical transformation by the Carbon-Bond Kinetics Mechanism. The amount of ozone produced by the mechanism depends on the rate of the nitrogen dioxide photolytic cycle, which in turn is mediated by the rate of free radical cycling associated with the oxidation of hydrocarbon compounds. Depending on their molecular structure, individual hydrocarbon compounds are represented by one or

more of five carbon-bond types. Distinguished by their different reaction rates and pathways, these carbon-bond types serve as surrogates for the complex mixtures of hydrocarbons found in the urban atmosphere. Simulations are typically carried out for 12 to 16 hours beginning at 0400 or 0500 LST, although multi-day simulations have also been conducted.

Primary inputs to the SAI Urban Airshed Model are point and area source emission schedules for seven species (NO, NO_2 and five carbon-bond types), initial and boundary concentrations both at the surface and aloft for eight species (seven emitted plus O_3), and a variety of meteorological data. These include a three-dimensional wind field, mixing depths, solar radiation (expressed as equivalent NO_2 photolysis rate), surface temperature, and exposure class, the latter an indicator of thermal instability.

The SAI Urban Airshed Model was developed by Systems Applications, Incorporated (SAI) under the sponsorship of EPA's Office of Research and Development. A more complete description of the model is found elsewhere (Layland, 1980). Besides the actual simulation program, the model is provided with a host of preprocessor programs which simplify input preparation.

Two versions of the simulation program were employed during these studies. The earlier version was used in the Tulsa and Los Angeles studies. It contained a numerical technique for advective transport which upon subsequent testing exhibited some undesirable properties. For this reason, the numerical technique was replaced with another that

is more accurate and generates less "numerical diffusion." This technique, which tends to give somewhat higher peak concentrations, was incorporated in a later version that was used in the Denver and St. Louis studies. The Denver study also compared the later version to the earlier version. All studies used the CBM II version of the Carbon-Bond Mechanism. However, substantial differences exist in the preprocessor programs used in the four studies due, in part, to differences in the availability of input data.

3. DESCRIPTION OF THE STUDIES

3.1 Tulsa

The Tulsa study was conducted under contract by Systems Applications, Incorporated. The study is described in a draft report by Reynolds et al. (1982). The results have been summarized by Layland et al. (1983).

The air quality and meteorological data required for modeling were obtained through a special field study conducted by Research Triangle Institute (Eaton et al., 1979). Monitoring stations were established for the collection of continuous measurements of ozone, NO_x, total nonmethane hydrocarbons, and winds. Data from ten ozone monitors at both urban and outlying sites were available for model evaluation. Hydrocarbon species data were also collected at the surface and aloft. In addition, aircraft measurements were taken of ozone concentrations aloft.

The emissions data were assembled by Engineering-Science (1980) from information obtained from the Tulsa City-County Health Department and the Tulsa Metropolitan Area Planning Commission. The basic emission rates were developed from stationary source records, transportation modeling of motor vehicle emissions, and per capita emission factors for miscellaneous sources.

A total of four days were modeled. The impact of emission reductions was examined on two of the four days. Measurements aloft were generally not available on the days modeled. For ozone, morning surface measurements at rural sites were selected to provide an indication of ozone aloft on each day. For hydrocarbons, a typical vertical profile was established for all days based on available aircraft measurements. Twice daily upper air soundings taken at a National Weather Service station in Oklahoma City were used to derive winds aloft and mixing depths. However, the modeling domain was limited to 1000 meters regardless of the afternoon mixing depth. Surface winds were interpolated from surface measurements and were smoothed to reduce divergence. NO_2 photolysis rates were derived empirically from hourly, surface-based, total solar radiation measurements on each day.

3.2 Denver

The Denver study was conducted at the National Center for Atmospheric Research (NCAR) under a cooperative agreement with EPA. The study grew out of earlier studies by Systems Applications, Incorporated, using an earlier version of the SAI Urban Airshed Model. The results of the NCAR study have been presented in a report by Dennis et al. (1983).

Only routinely collected meteorological and air quality data were available for the study. No monitoring data existed from which early morning levels of ozone and precursors transported into the modeling region or accumulated overnight could be estimated. Five ozone monitoring sites, located within the urbanized area of Denver, were available for model evaluation. No outlying sites had been established to measure afternoon levels

of ozone associated with emissions transported beyond the immediate urban area. No aircraft measurements were taken.

The emissions data base was assembled by the Colorado Department of Health from stationary source records and motor vehicle travel records.* The latter were derived from transportation modeling conducted by the Denver Regional Council of Governments. Emissions from miscellaneous area sources were also included. Although the base year inventory for the study was 1979, a second earlier inventory for 1976 was developed, using the same techniques, for the purpose of air quality trends analysis.

Simulations were performed for eleven days. Additional simulations were run for a subset of eight days using the earlier inventory. Since no air quality measurements aloft or at outlying sites were available, typical urban background values were assumed for all eleven days. Twice daily upper air soundings routinely made at Stapleton International Airport and tower data taken at Boulder Atmospheric Observatory provided information on winds aloft. Surface winds were obtained by interpolation from surface measurement sites. Mixing heights were derived from the Stapleton soundings. However, the modeling domain was limited to 1300 meters regardless of the afternoon mixing depth. NO_2 photolysis rates were based on theoretical, clear sky rates rather than solar radiation measurements because these were unavailable. The photolysis rates were adjusted from sea level to the ground level elevation of Denver.

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*One large power plant, Cherokee, was eliminated from the data base due to problems in treating such a concentrated source of NO_x emissions in the model.

3.3 St. Louis

The St. Louis study was conducted jointly by EPA's Office of Research and Development and the Office of Air Quality Planning and Standards. Initial development of the model inputs was done under contract by Systems Applications, Incorporated. Study results have been described in two reports (Schere and Shreffler, 1982 and Cole et al., 1983) and a summary paper (Cole et al., 1982).

The extensive Regional Air Pollution Study (RAPS) in St. Louis provided the emissions, air quality, and meteorological data needed for modeling (Strothmann and Schiermeier, 1979). Ozone, NO_x, total nonmethane hydrocarbons, winds, and temperature measurements were taken continuously at both urban and outlying sites. Data from 25 ozone monitors were available for model evaluation, mostly within the urbanized area of St. Louis. An intensive program of upper air soundings was also included as part of the RAPS program. In addition, an instrumented helicopter provided measurements of ozone concentrations aloft. Although samples were collected, valid hydrocarbon species data were unavailable, either at surface sites or aloft.

The RAPS point source inventory was developed by EPA directly from questionnaires, plant visits, stack tests, and other available information. A detailed transportation data base was developed from which motor vehicle emissions were derived. Emissions from miscellaneous area type sources were developed using techniques based on economic activity and population.

Simulations were performed for twenty days. Additional simulations for a subset of three days were conducted to examine emission

control strategies. Since ozone measurements aloft were not always available on the days modeled, morning surface measurements at rural sites were selected on each day to represent ozone aloft. For hydrocarbons and NO_x aloft, a single set of background values was assumed for all twenty days. The wind field was generated by a simple boundary layer model which used the surface temperature measurements to perturb the mean boundary layer flow. Mixing heights were estimated from upper air soundings. NO_2 photolysis rates were empirically derived from continuous surface-based total solar radiation measurements for each day. These were then adjusted using radiative transfer theory to provide layer-averaged rates.

3.4 Los Angeles

During the development of the SAI Urban Airshed Model, numerous applications were conducted in Los Angeles. The model, as originally formulated, was tested on six days in September, October, and November, 1969 (Reynolds et al., 1973). Numerous refinements in both physical and chemical treatments were made subsequently. Later model applications focused on two days, June 26, 1974 and August 4, 1975. These applications were originally sponsored by several organizations, including the California Department of Transportation, the California Air Resources Board, and Southern California Edison Company. The June 26, 1974 simulation was extended to include the following day, June 27, in a study sponsored by the U.S. Department of Transportation. The results from these studies were later updated in several studies, one sponsored by EPA, and others by Southern California Edison Company and the Western Oil and Gas Association. The latter study also included a second two-day episode, November 7 and 8, 1978. The EPA study focused on the sensitivity of the

model predictions to the availability of detailed data for constructing model inputs (Tesche et al., 1981). Only the results from the most recently performed studies are discussed in this report.

Historically, ambient monitoring in Los Angeles has been quite extensive. Considerable information was therefore available to characterize air quality and meteorological conditions for the purpose of modeling. More than forty monitoring stations provided surface measurements of O_3, NMHC, and NO_x. Nineteen to twenty-five ozone monitors were available throughout the Los Angeles basin on different days for use in model evaluation. An extensive hydrocarbon species monitoring program had been carried out during the summers of 1974 and 1975 which provided detailed information on the composition of ambient hydrocarbons. In addition, special studies had been conducted which involved airborne sampling of O_3 and NO_x. Upper air and acoustic soundings were available for as many as six locations at various times during the day. Numerous stations provided measurements of surface winds.

Emissions from major stationary sources were derived from records maintained by the South Coast Air Quality Management District. Nonhighway area source emissions were developed by the Southern California Association of Governments based primarily on demographic data. Highway motor vehicle emissions were prepared using the transportation modeling approaches developed by the California Department of Transportation and the California Air Resources Board.

As indicated above, recent simulations have been performed on five days.* In order to establish background concentrations, both at the surface and aloft, surface measurements at outlying stations and on elevated terrain were used, together with special airborne monitoring data. Nighttime shear-driven mixing depths were derived from surface wind speeds and acoustic soundings. Daytime convective depths were based on temperature soundings. In order to represent the effects of terrain channeling and the diurnal sea breeze on pollutant transport, a three-dimensional model was used to develop the wind field. The study used theoretical, clear sky NO_2 photolysis rates. These were adjusted to account for aerosol scattering and altitude above ground.

*Although control strategy simulations have been performed for Los Angeles, those carried out using the more recent versions of the model have been conducted under private auspices or the results are otherwise unavailable for inclusion in this report.

4. EVALUATION OF MODEL PERFORMANCE

If one could be assured that all model inputs are correct, the accuracy and precision of a model could be determined by comparing the model predictions with the observed values. However, the SAI Urban Airshed Model requires a large number of inputs that are difficult to specify. Thus, the model performance evaluation tests the application as well as the model itself. Errors related to model deficiencies and errors induced by designation of model inputs are difficult to distinguish.

In a broader sense, the evaluation of the performance of a model, such as the SAI Urban Airshed Model, really tests whether air quality observations can be explained based on available information and understanding of the physical and chemical processes involved. If they cannot, then one's understanding of the problem is incomplete. Either the emissions are incorrect, the significance of background pollutant levels is misjudged, the meteorological conditions are inadequately portrayed, or turbulent diffusion or chemical transformation is improperly represented. Alternatively, the air quality measurements could be in error. The integration of information from disparate sources in a quantitative model can draw attention to needed refinement in any one or more of these areas.

Another limitation is that information available to evaluate model performance is always incomplete. One of the findings of the St. Louis study is that a large number of days are required to fully assess model performance due to a large degree of day-to-day variation in model prediction errors. Results from the Tulsa and Los Angeles studies are limited to a small number of days. Only the St. Louis and Denver studies have a sufficient number of days to characterize the range of performance likely to be encountered. However, even in these studies there are limitations in the spatial coverage of air quality monitors. As indicated in Chapter 6, only in the Denver study was an attempt made, using limited data, to evaluate the ability of the model to predict the effect of emission reductions on ambient ozone levels.

It should be noted that evaluation of model performance is complicated by the absence of a "standard" version of the SAI Urban Airshed Model. In Chapter 2, a distinction was drawn between two versions of the model, one brought about by a major revision to the simulation program. In addition, different users have tended to make various other changes to the model, particularly the preprocessor programs. In this sense, the model has continued to evolve. Thus, comparisons among the four studies are difficult to assess.

In a similar vein, the approach taken by the investigators toward simulating the days varied among the four studies. In the Los Angeles and Tulsa work, a relatively few number of days were simulated. Attempts were made to optimize the performance of the model, within the confines of the available data. In the Denver and St. Louis studies,

a much larger number of days were simulated and much less attention was given to any particular day.

4.1 Peak Accuracy

Assessment of peak accuracy often receives the greatest attention in model evaluation studies since implementation of emission controls is predicated upon reducing the maximum daily ozone in the region to the level of the standard. Various measures of peak accuracy have been proposed. The most useful measures appear to be those which (1) use predicted values at air quality monitoring stations only and (2) do not require a rigid pairing in time and space between predicted and observed concentrations.

The rationale for the first criterion is that the alternative, use of the all-grid daily maximum prediction, tends to bias the evaluation toward overprediction. This is because the daily maximum prediction, which is selected from the entire modeling region, has a much greater probability of capturing the actual peak concentration than does a monitoring network having a limited number of monitors. The second criterion recognizes that pairing the observed and predicted concentrations based on the time and/or location of the observed peak tends to bias the evaluation in the opposite direction, toward underprediction. This is related to the sparsity of the monitoring network and the nonrandom selection of the days chosen for modeling. Dennis et al. (1983) offer a further discussion regarding this aspect of the model evaluation problem. Although pairing of observed and predicted concentrations is common practice, this approach to model evaluation, besides its potential for causing a

misleading or biased evaluation, fails to recognize that prediction of the exact time and location of the peak concentration, in a regulatory context, is of lesser importance than the prediction of the magnitude of the peak.

Criteria (1) and (2) above have been observed in making the scatter diagram for St. Louis shown in Figure 1. In this diagram, the predicted and observed peaks are paired only by day (not by hour or site) and the predicted peaks are restricted to monitoring sites. Apparent from this diagram is some tendency for the model to underpredict peak ozone at the locations of the monitoring sites. However, most of the predicted maxima fall within ± 30 percent of the observed maxima.

The same presentation is made in Figure 2 for Denver. The tendency towards underprediction of peak ozone is quite pronounced. Note that all the predicted daily peaks are less than the corresponding observed peaks. On average, the daily peak ozone is underpredicted by about 30 percent.

The relatively small number of days modeled in Los Angeles and Tulsa limit what can be concluded from these studies. However, the results from these may be combined with those of Denver and St. Louis in order to see how well the observed peaks are reproduced for the ensemble of studies. In principle, the larger the number of studies, the more one can distinguish errors associated with particular applications and deficiencies that are inherent in the model itself. However, to the extent that methods for developing model inputs are common to all studies, systematic errors in the

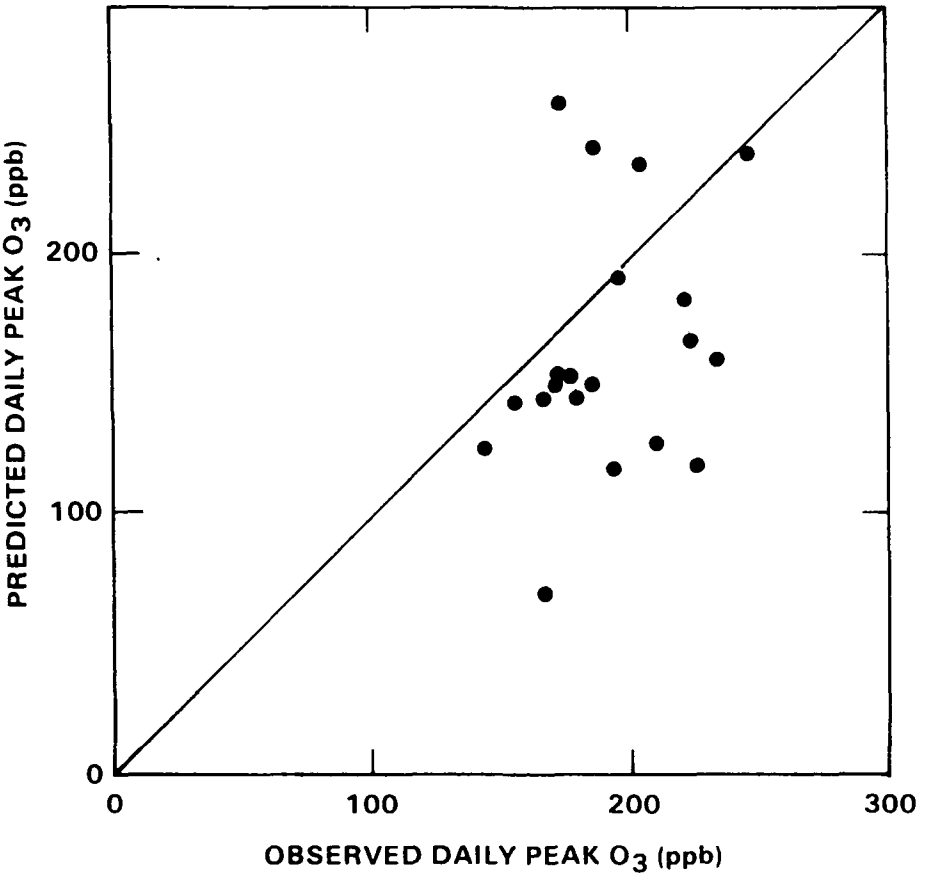

Figure 1. Daily peak observed and predicted ozone for St. Louis.

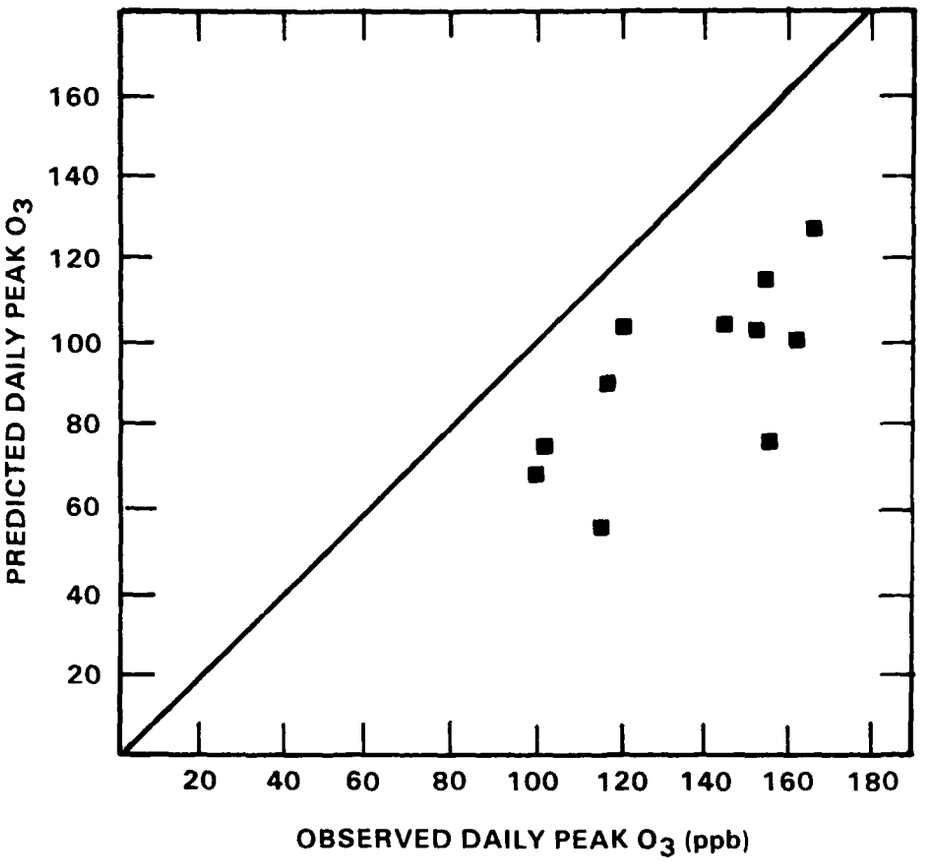

Figure 2. Daily peak observed and predicted ozone for Denver. (Adapted from Dennis et al., 1983)

predictions may simply reveal deficiencies in the methods. Unfortunately, as was pointed out earlier, neither the models nor the methods were identical.

Having acknowledged the limitations of direct comparisons among studies, observed and predicted daily peak O_3 for all four cities are presented together on a scatter diagram in Figure 3. Although the forty points show an overall tendency toward underprediction, about three-quarters of the predicted maxima fall within ± 20 percent of the observed peaks. The results in Figure 3 also indicate the SAI Urban Airshed Model can give reasonably accurate estimates of peak ozone over a wide range of concentrations (10 to 35 pphm). The points above the line, while in the minority, show that either overestimation or underestimation are possible outcomes. However, the results suggest the Denver application was affected by unique deficiencies in critical inputs or model treatments.

4.2 Overall Accuracy

While the assessment of peak accuracy is essential, model accuracy at lower concentrations is also important. Demonstrating accuracy across the full range of values helps to establish the validity of the model's treatment of physical and chemical processes and therefore gives greater confidence in the reliability of the model's predictions when used for estimating control requirements.

The most extensive analyses of model accuracy are the St. Louis and Denver studies. A concise summary of the findings for the twenty day St. Louis study is given in Figure 4. In this figure, model accuracy on each day is expressed as the daily mean residual (or bias, $\overline{O-P}$) for all

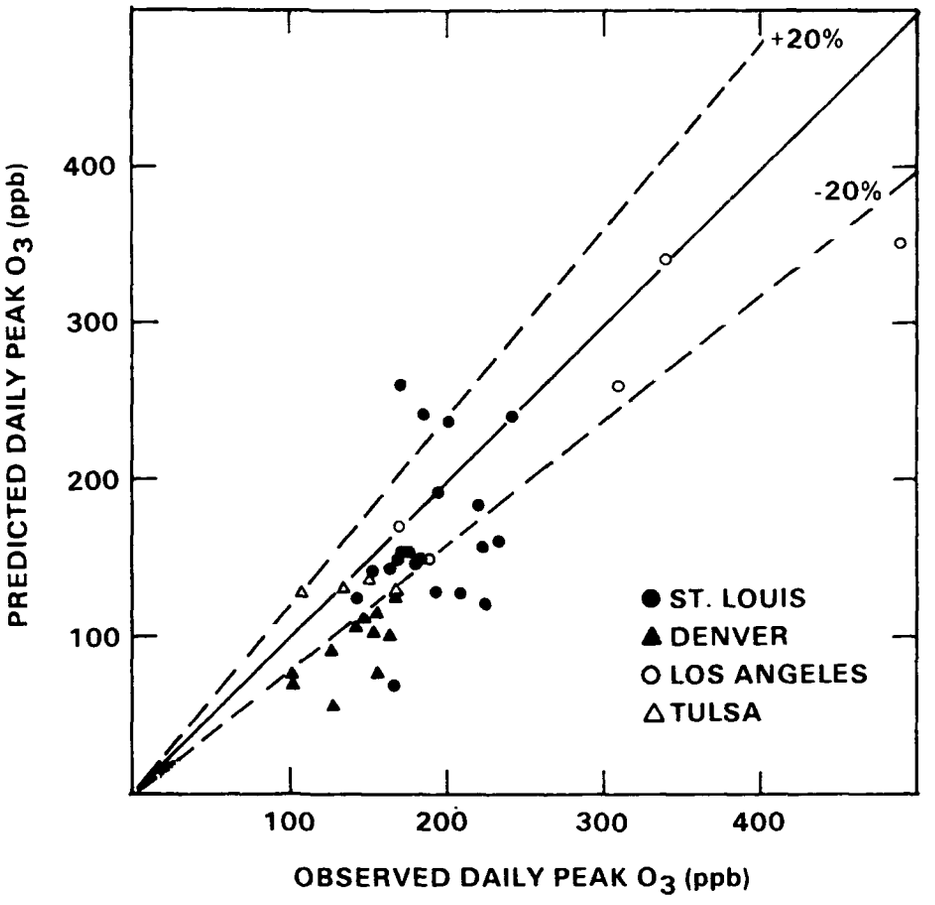

Figure 3. Scatter diagram of peak ozone for four cities.

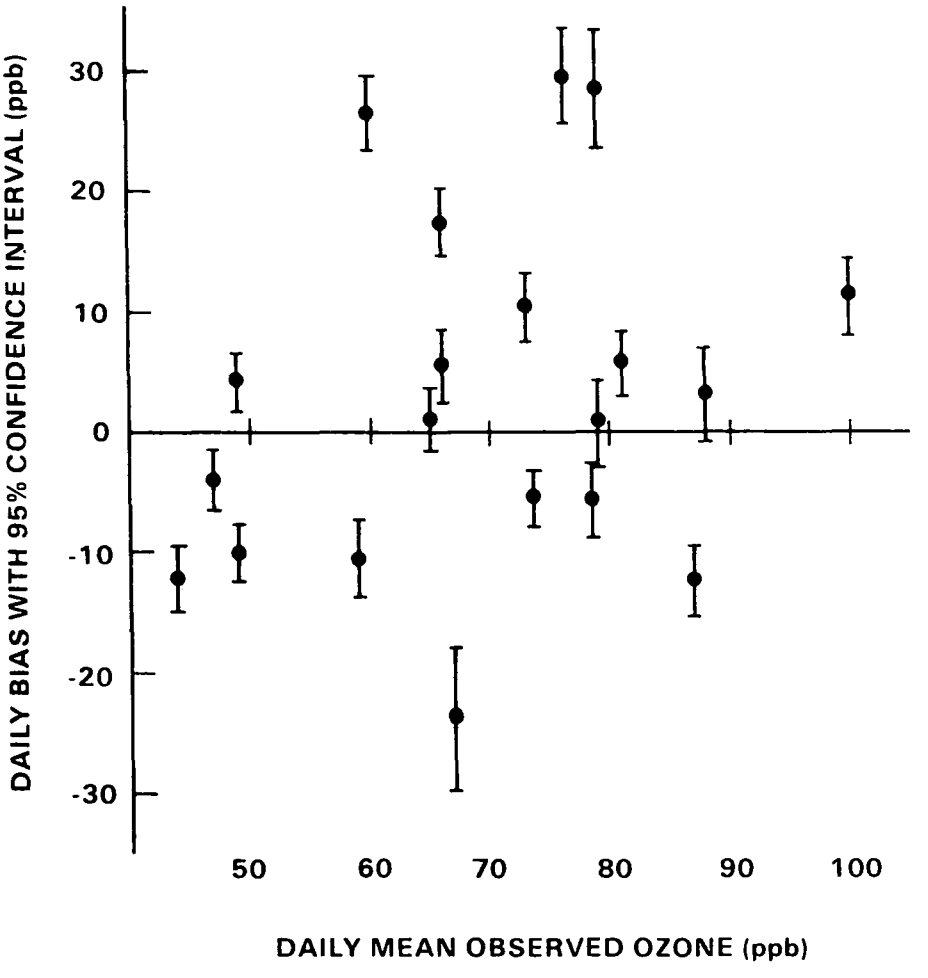

Figure 4. Daily mean bias for St. Louis without autocorrelation.

pairs of observations and predictions.* An estimate of the precision of the bias statistic is indicated by the 95 percent confidence interval, which is also shown in Figure 4. These confidence intervals represent a lower limit, since autocorrelation was not considered in their computation. Considering the entire set of twenty days, no overall bias is evident. Moreover, there is no pattern in the daily mean residual with respect to the daily mean observed ozone.

A similar presentation of the daily mean bias for the eleven days in Denver is made in Figure 5. The confidence intervals are quite wide due to the few numbers of observation sites and because autocorrelation was considered. Although for most days, individually, the bias is not significantly different from zero (the confidence interval includes the zero value for the bias statistic, $\overline{O-P}$), the ensemble of days clearly shows underprediction.

The overall accuracy of model predictions for any one day is best ascertained from a scatter diagram of all pairs of observations and predictions. Two individual days are shown for St. Louis in Figures 6 and 7, August 18, 1975 and July 13, 1976. On both days, there is a shift toward underprediction at higher concentrations. Of the two, August 18 shows the greater underprediction at higher concentrations, yet the daily mean residual, -12.3 ppb, indicates overprediction. In contrast, the daily mean residual for July 13 is +5.9 ppb. From Figure 7, the sizeable negative mean residual on August 18 is clearly

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*It should be noted that the daily mean residual can be a misleading indicator of the overall accuracy of the model, as illustrated later on.

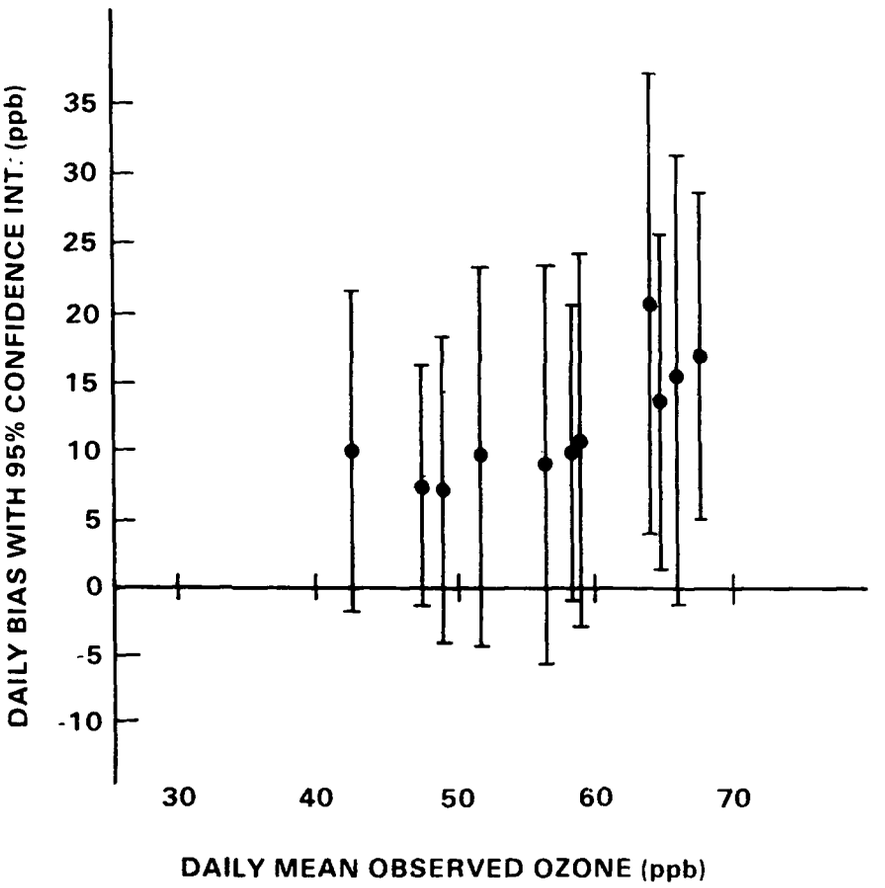

Figure 5. Daily mean bias for Denver with autocorrelation. (Adapted from Dennis et al., 1983).

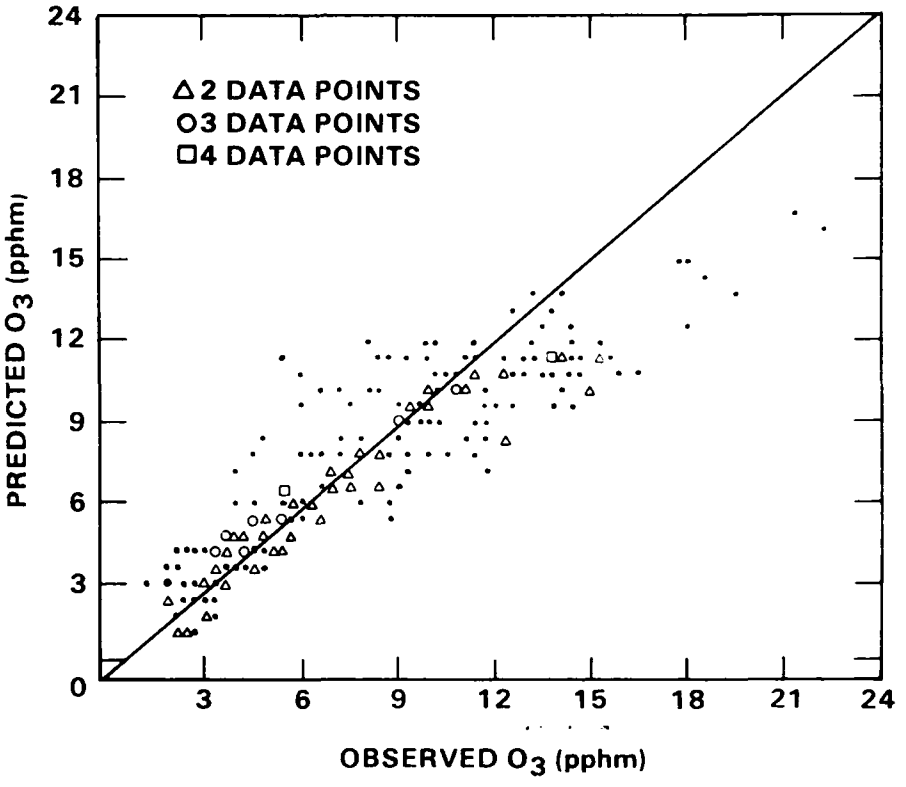

Figure 6. Scatter diagram for July 13, 1976, St. Louis

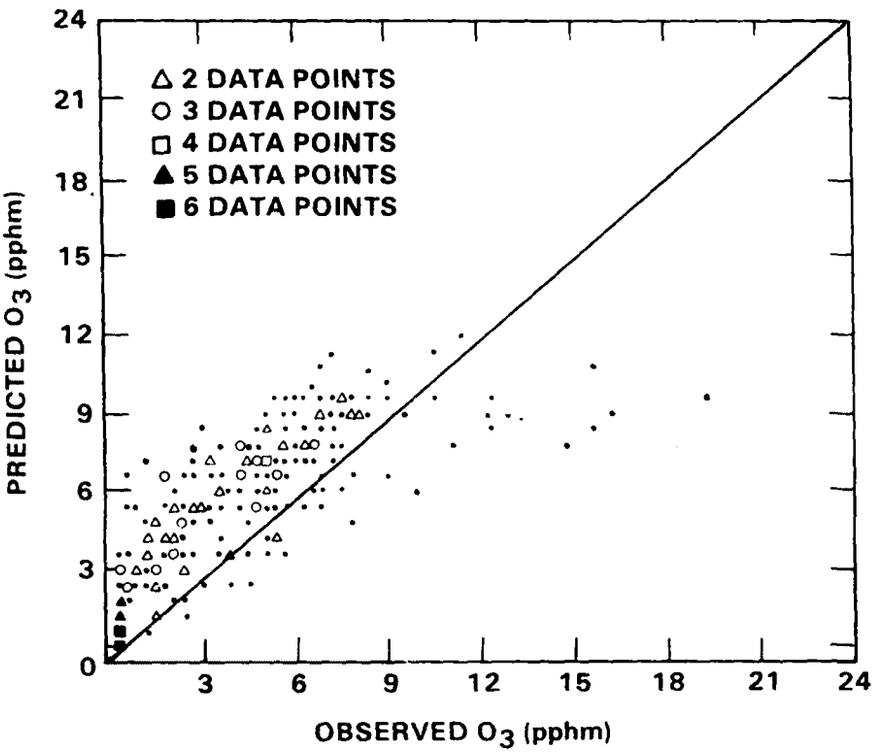

Figure 7. Scatter diagram for August 18, 1975, St. Louis.

attributable to the large number of overpredictions below 100 ppb observed. Thus, the daily mean residual, by lumping together all pairs of observations and predictions, is a relatively poor indicator of the overall accuracy of the model on any one day.

A tendency toward underprediction at high concentrations is expected because the sample of days chosen for modeling was not a random sample. Days were selected because high ozone concentrations had been observed at monitoring sites. In St. Louis, the spacing between ozone monitors over a considerable part of the modeling region is large compared to the size of the urban plume. Thus modest errors in the spatial alignment of the predicted plume will lower the predicted concentration at the monitor which had experienced high concentrations without appreciably raising the predictions at another monitoring site: This predisposes the outcome towards underprediction. Indeed, a shift toward underprediction at high ozone concentrations is apparent on fifteen of the twenty test days. On only one day is there a shift toward overprediction at high concentrations. Though the problem of nonrandom sampling no doubt exerts an effect on the results, it does not by itself explain the degree of underprediction on at least eight of the fifteen days on which the peak ozone concentration is underpredicted in the St. Louis study. On these days, the all-grid daily maximum prediction is less than the daily maximum observation.

Scatter diagrams for July 29, 1977 and August 3, 1977 in Tulsa are shown in Figures 8 and 9. On August 3, 1977, monitoring coverage was excellent in the area where the urban plume was located. On this day,

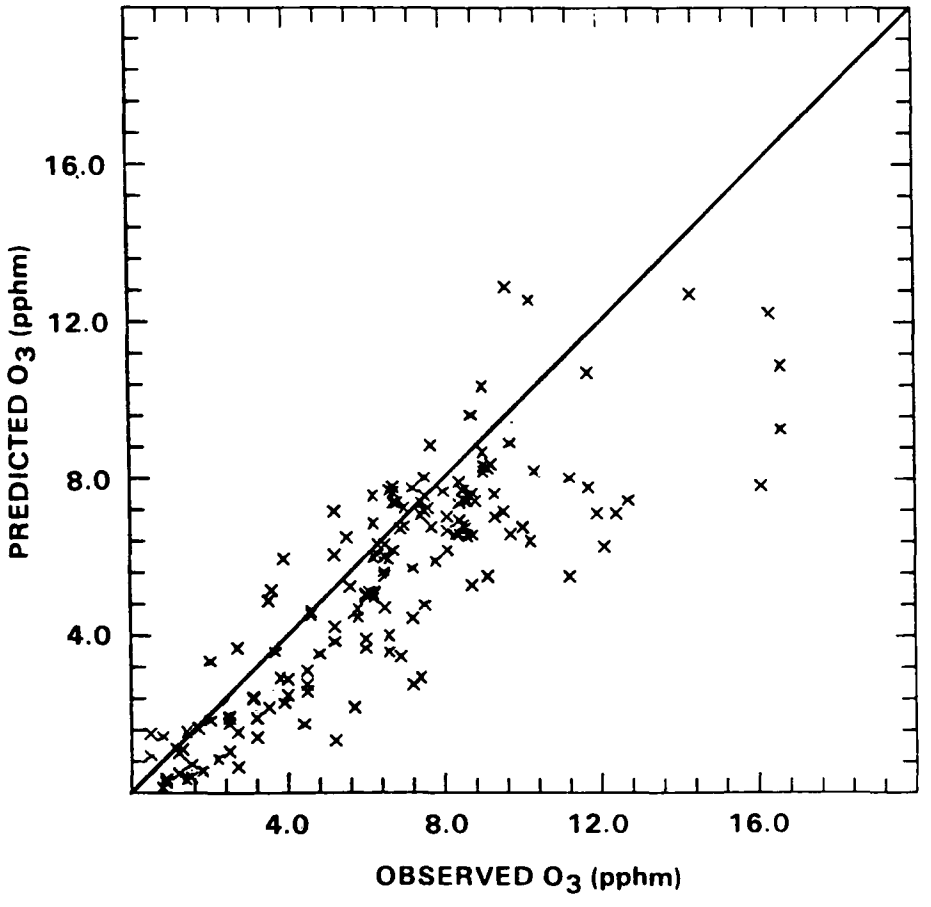

Figure 8. Scatter diagram for July 29, 1977, Tulsa (Courtesy of Systems Applications, Inc.).

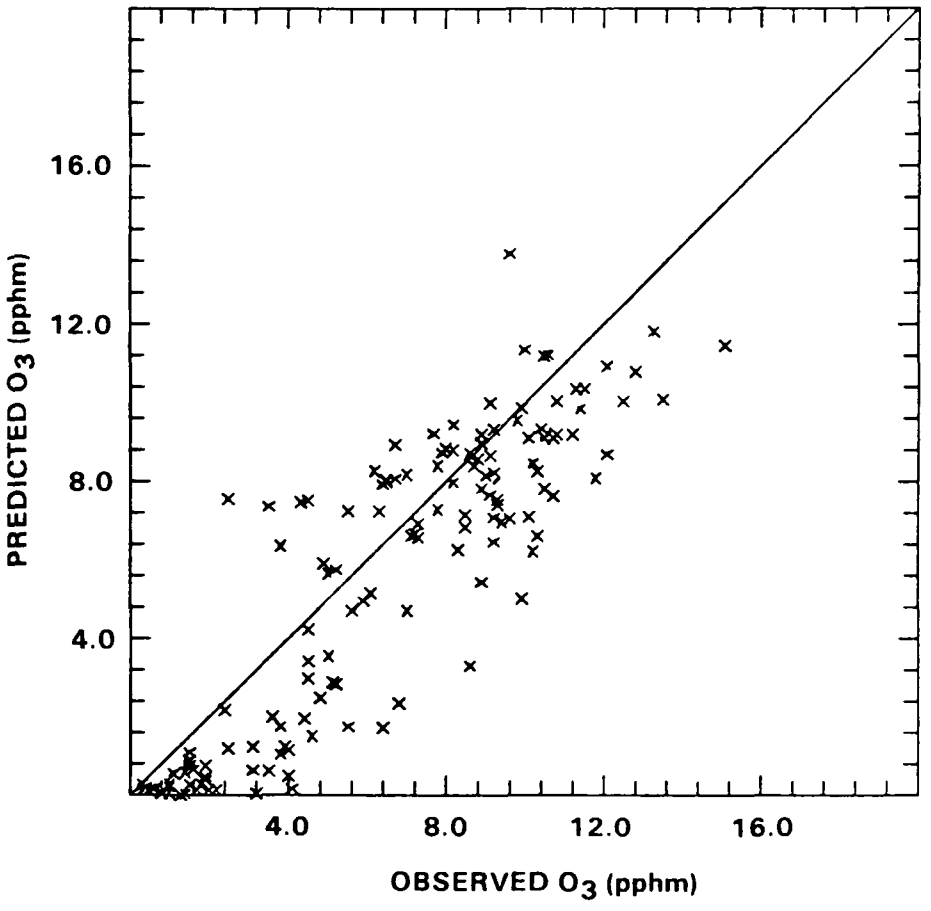

Figure 9. Scatter diagram for August 3, 1977, Tulsa (Courtesy of Systems Applications, Inc.)

little underprediction is apparent in Figure 9. In contrast, underprediction at high ozone concentrations is seen in Figure 8 for July 29, 1977. In this case, however, no monitors were located where the high ozone concentrations were predicted to be. In addition, the highest ozone concentrations (those greater than 16 pphm) are associated with a monitor that was calibrated using the NBKI technique, a technique shown in an intercomparison study to give results that were high by 25 percent.

Of all the studies, Los Angeles has the clear advantage of having more ozone monitors more evenly distributed. Scatter diagrams for June 26 and June 27, 1974 are shown in Figures 10 and 11.* The results for June 26, 1974 show a slight tendency toward overprediction across the entire range of ozone concentrations. For June 27, 1974, no bias is apparent in the model predictions up to a concentration level of 40 pphm. However, the very highest concentrations, about 50 pphm, are underpredicted. This two day episode was recently resimulated using an improved numerical technique (see Section 2) but there was only modest improvement for the highest two observations. While underprediction at these very high concentration levels could have any number of causes, some material may have been inadvertently lost from the modeling region when the winds shifted offshore at night, material that would otherwise have been advected inland again on the following day, June 27.

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*It should be noted that the observed ozone concentrations in these figures have been adjusted to account for differences in calibration techniques for the various monitoring stations. Specifically, ozone concentrations measured at monitors calibrated with the NBKI technique were lowered by 22 percent.

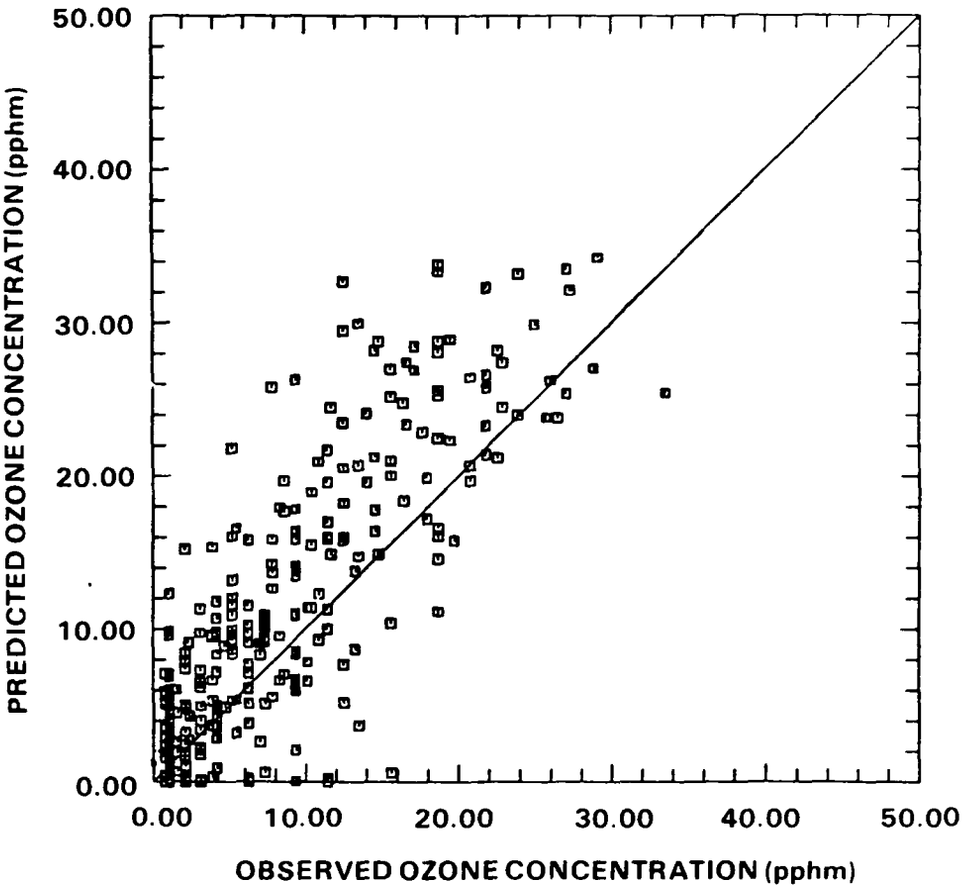

Figure 10. Scatter diagram for June 26, 1974, Los Angeles (Courtesy of Systems Applications, Inc.).

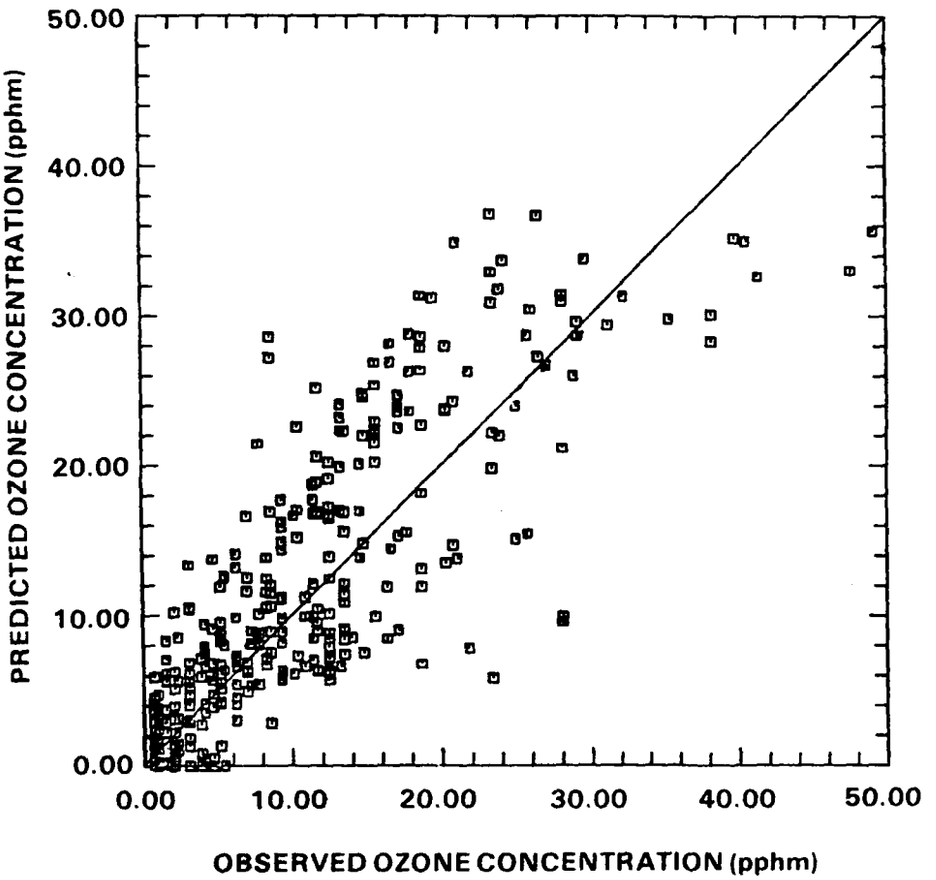

Figure 11. Scatter diagram for June 27, 1974, Los Angeles (Courtesy of Systems Applications, Inc.).

4.3 Spatial and Temporal Patterns

In addition to peak accuracy, in an unpaired sense, and overall accuracy, another aspect of model accuracy is the replication of spatial and temporal patterns. The success of the model at replicating these patterns hinges on its ability to predict ozone concentrations at a particular time and location. This is a rigorous requirement for any model.

Very generally speaking, spatial patterns tend to be controlled by the wind field and temporal patterns tend to be controlled by sunlight intensity, in the absence of major perturbations in other model parameters. However, a distinction between spatial and temporal patterns is partly an artificial one. Pollutant transport and reaction kinetics are interconnected. A significant error in the timing of the ozone build-up necessarily carries over and influences the location of the peak ozone concentrations. Nevertheless, examining spatial and temporal patterns can be useful for further evaluating model performance.

The ability of the model to reproduce the spatial and temporal patterns of ozone is difficult to judge from calculated spatial and temporal correlation coefficients. The temporal pattern of ozone production is so highly correlated with sunlight intensity that most any reasonable diurnal pattern of sunlight intensity leads to high temporal correlation coefficients, on average. Although time series of predictions do not necessarily closely follow the observations, the two are found to be in phase when the results for all days are averaged, as seen from the results of the St. Louis study in Figure 12. At any particular station, the temporal pattern can be strongly influenced by the wind field, which can move

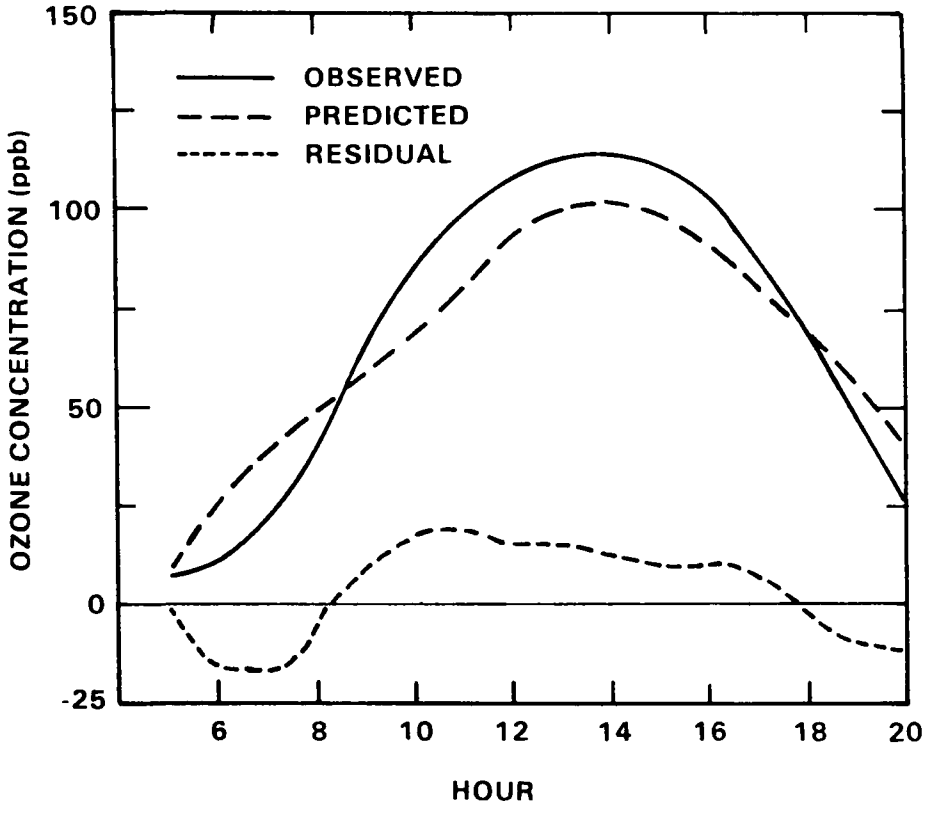

Figure 12. Comparison of 20 day, all station average time series of observations and predictions for St. Louis.

the urban ozone plume toward or away from the monitoring station, or by individual NO_x plumes, which can rapidly deplete ozone levels. By contrast, the spatial correlation coefficient is sufficiently sensitive to minor displacements in the location of the ozone plume that the resulting correlations are uniformly low. Low correlations are found even when visual inspection of spatial isopleths indicates fair to good agreement with the observation network.

For these reasons, direct visual inspection of time series plots and spatial isopleth maps offers the best opportunity for evaluating the ability of the model to reproduce temporal and spatial patterns. The two types of presentations are interrelated and should be examined in tandem to avoid misdiagnosis. Frequently, a problem in the temporal pattern at a particular monitoring station, as shown in a time series plot, can be caused by a simple displacement of the ozone plume. The latter may be apparent from a series of spatial isopleth maps. This kind of problem may be unrelated to either the chemical kinetics mechanism, the parameterization of turbulent diffusion, or the treatment of emission sources. Instead, it may be attributable entirely to errors in the wind field.

For control strategy purposes, the location and timing of the ozone plume is less important than the magnitude of the peak concentrations. As discussed previously, errors in the location of the plume may cause the model to appear to underpredict in relation to the observations at the monitoring locations. Visual inspection of spatial isopleth maps can help to identify if this is the major cause of the underprediction

or whether other factors may be involved on any particular day. Spatial isopleth maps can also help to identify possible causes of overprediction.

Despite the important effects of errors in the wind field, the results of the four studies indicate a general correspondence between the fields of observed and predicted ozone concentrations. However, results from both the Tulsa and St. Louis studies exhibit a tendency to underestimate the spatial extent of the ozone plume, i.e., the area of ozone concentrations elevated above regional background levels. This appears to be true even when the magnitude of the peak prediction agrees well with that of the peak observation. Evidence of this is necessarily qualitative, as exact comparisons are impossible, given a sparse observation network.

4.4 Conclusions

From the results of the four studies, a number of general conclusions can be reached regarding how the SAI Urban Airshed Model can be expected to perform and the methods by which it can be evaluated. These are as follows:

- The accuracy of the model predictions can be expected to vary greatly from one simulation day to the next, even on days with similar levels of detail in input information. This is evident from each of the four studies.
- The accuracy of the model predictions can also be expected to vary considerably from one study (i.e., city) to the next, depending in part on the availability of input information and in part on the methods by which it is prepared for input to the model. For example, model predictions in Denver show significantly less accuracy than those in Tulsa, St. Louis, or Los Angeles.

- Overall, the model results have been shown to exhibit a tendency toward underprediction. However, this is judged to be a serious problem in only one of the four studies (i.e., Denver). It is unclear whether the cause is related to inadequacies in the input information or in the model itself. There is no strong evidence that other applications with other data bases would necessarily exhibit the same tendency.

- Determining the accuracy of the model predictions is an inexact science. Simple statistical representations of model performance (e.g., the mean residual, the root mean square error, or the correlation coefficient) can be expected to provide limited insight into the ability of the model to predict the maximum ozone concentration, the concentration used as a design value for control strategy analysis.

- In gauging the accuracy of the model at predicting peak ozone concentrations, rigorous pairing of the observations and predictions in time and space has the effect of causing the model to appear to underpredict. This is related to the sparsity of the network of observations and the nonrandom selection of days for model evaluation. In contrast, direct comparison of the daily maximum prediction (all grid maximum) to the daily maximum observation (all station maximum) has the effect of causing the model to appear to overpredict. This is related to the different sample sizes from which the maximum concentrations are drawn. Therefore, undue reliance on either of these comparisons is not recommended, although together they do serve to establish probable bounds on the true accuracy of the model predictions.

- Due to problems brought about by rigorous pairing of observations and predictions, statistical approaches to model evaluation require subjective interpretation in order to judge the accuracy of model predictions of peak concentrations on any given simulation day. Users may find that spatial isopleth maps and time series plots are useful tools for making these interpretations.

- Scatter diagrams of all pairs of observations and predictions serve to convey quickly the major features of the overall predictive capability of the model on any given simulation day. Scatter diagrams are highly recommended for this purpose.

5. MODEL SENSITIVITY

Given that the predictions of the SAI Urban Airshed Model, like those of other models, have less than perfect accuracy, it is useful to consider what factors contribute significantly to errors in the model predictions. During the development and application of the model, a variety of testing has been conducted to evaluate the importance of various model inputs and to identify those to which the model predictions are most sensitive. Only the results of the studies discussed in Section 3 are considered here. Results from other studies using earlier versions of the model are considered less reliable. Presumably, refinements in the specification of these inputs, or greater availability of information upon which they are based, will lead to more accurate predictions, at least in the absence of serious deficiencies in the model itself.

5.1 Background Air Quality

Assumptions regarding background air quality appear to have significant effects on ozone predictions. These assumptions are reflected in the model inputs for initial and boundary concentrations, both aloft and at the surface. When reactive hydrocarbons aloft were reduced by a a factor of two in the Tulsa study, from 84 to 42 ppb C at 500 meters altitude, the maximum predicted ozone concentration was reduced by 17 percent. Oxygenated organics were also reduced in this test from 12 to 4 ppb C. Similar tests were conducted on two days in the Denver study. On both

days, reactive hydrocarbons aloft and at the boundaries of the modeling region were reduced from 52 to 19 ppb C and oxygenated organics from 5.0 to 1.2 ppb C. For the day on which the maximum ozone was observed within the urban area, the effect was negligible. However, on the day when the urban ozone plume was transported outside the urban area, the maximum predicted concentration was lowered by 12 percent. In the Los Angeles study, use of total NO_x measurements and an assumed HC/NO_x ratio of 7 for establishing initial concentrations for hydrocarbons, instead of actual hydrocarbon species measurements, was found to lower ozone concentrations above 12 pphm by an average of 40 percent.

The effect of background ozone has been examined in the Denver study. A change from 2 pphm to 9 pphm increased the maximum ozone prediction by an equal amount on several days. Even on the day having the highest ozone concentrations, the maximum prediction was increased nearly 4 pphm.

The importance of background depends on the wind field and the mixing which ensues with higher wind speeds and greater vertical wind shear, as well as on the rate of growth of the mixed layer. Of course, background air quality becomes more important, in a relative sense, as emissions are reduced. Better measurements of background concentrations of ozone and the whole array of ozone precursors are necessary to improve the accuracy of model predictions.

5.2 Solar Radiation

The accumulation of ozone in the polluted troposphere is caused by the photodissociation of nitrogen dioxide which in turn is driven by

solar radiation. The accurate specification of NO_2 photolysis rates is therefore essential to the accurate prediction of ozone concentrations. At equilibrium, ozone concentrations should be directly proportional to the NO_2 photolysis rate, in the absence of hydrocarbons. Tests conducted in the St. Louis study show that although the maximum ozone prediction is slightly less sensitive than this, the relationship between NO_2 photolysis rate and peak ozone is only marginally less than one-to-one.

The use of theoretical, clear sky, ground level photolytic rates may not accurately reflect the true photolytic rates in urban atmospheres at a particular time and location. Ground level rates understate the true photolytic rates aloft due to the attenuation, near the surface, of short wave radiation by ozone absorption and aerosol scattering, resulting in lowered ozone predictions at the surface. Scattering by clouds can significantly alter both the intensity and spectral distribution of sunlight, thereby either enhancing or depressing photolytic rates, depending on cloud cover and solar angle. The inability to explicitly consider radiative transfer in the model, or simply to provide vertically varying photolysis rates on input, consequently places a limitation on the accuracy with which ozone concentrations can be predicted.

5.3 Vertical Mixing

Vertical mixing has a strong effect on model predictions. These effects are partly associated with the impact which background concentrations aloft and elevated emissions, above the morning mixed layer, have on surface concentrations as the afternoon mixed layer develops. The extent of vertical mixing is controlled jointly by three principal user-specified

inputs: (a) vertical grid spacing, (b) mixing height/region top, and (c) exposure class. Vertical grid spacing is important because mixing is assumed to be instantaneous within any grid cell on a time scale comparable to the time step used for numerical integration. Specification of the mixing height/region top places a lid on the mixed layer. The exposure class, in combination with wind speed, determines the vertical eddy diffusivity at the grid mesh points. Although vertical eddy diffusivity is a complex function involving several parameters, exposure class is the most important, independently controlling parameter. Given the importance of vertical mixing, and the interrelationships between the various user-specified inputs, careful attention must be given to the way in which these inputs are established, within the context of the theoretical framework of the model.

Tests conducted in the Denver and Los Angeles studies on vertical grid spacing produce conflicting results. This is likely associated with interactions with other model inputs which differ for the two studies. In the Denver study, when the grid spacing in the mixed layer was increased from 250 to 330 meters at midday, ozone concentrations were reduced up to 24 percent at one station, while the daily maximum was reduced 8 percent. Little effect from vertical grid spacing was seen for the Los Angeles study. However, the Los Angeles work demonstrates very clearly the importance of pollutants which reside in the layers aloft, below the region top but above the morning mixed layer. When the aloft layers were eliminated, large increases or decreases were seen at individual stations, although the daily maximum ozone concentration was reduced only 5 percent. In some cases, surface ozone concentrations more than doubled, due to the removal of NO_x emissions emitted into the layers aloft, thereby eliminating ozone

scavenging which would otherwise have taken place when the emissions were mixed to the surface later in the day.

The specification of mixing height/region top is also tied to the entrainment of pollutants from aloft. Results from both the Denver and St. Louis studies show that an increase in afternoon mixing height/region top, in the range of 25 to 30 percent, actually caused a small increase in surface ozone concentrations, indicating that entrainment was more important than dilution. At the same time, a decrease of 25 percent in the mixing height in the St. Louis study also increased the daily maximum ozone prediction, by an amount that was much less than, or equal to, the increase expected from a simple box model treatment of dilution in the absence of chemical reaction.

Exposure class is used in the model, as indicated previously, to categorize the thermal instability of the atmosphere. Tests conducted during the Denver study reveal that the accuracy of model predictions is closely tied to the exposure class parameter. A modification to the exposure class that corresponds to a change from unstable to neutral stability increased peak ozone concentrations by as much as 38 percent at individual stations. The daily maximum ozone was increased similarly. Unfortunately, exposure class is a rather vaguely defined parameter, one that depends on solar radiation as well as surface heating, or temperature. Perhaps these would better be input to the model directly and, together with surface winds, be used to calculate the vertical eddy diffusivity, thereby avoiding the need for an exposure class parameter altogether.

It is interesting to note that the change in the exposure class improved the accuracy of the CO predictions in the Denver study. The CO predictions were low compared to the observations. However, CO measurements may not be a good yardstick for judging the adequacy of the treatment of vertical mixing. This is because high CO concentrations occur in localized "hot spots" which, on a spatial scale, are much smaller than the size of a typical grid cell.

5.4 Emissions Composition

A number of tests have been carried out to examine the effect on ozone predictions of changes in the chemical composition of emitted hydrocarbons and of emissions of oxygenated organic compounds. When a chemical composition typical of motor vehicle exhaust was used in place of a less reactive urban mixture, the daily maximum ozone prediction was increased in the St. Louis study by as much as 30 percent. A similar test in the Los Angeles study shows the daily maximum ozone prediction was little affected but ozone concentrations above 12 pphm were increased by as much as 14 percent, on average. At individual stations, increases ranged as high as 50 percent. In the St. Louis study, ozone predictions are particularly sensitive to emissions of organic oxygenates. An increase in the fraction of total emitted carbon which is oxygenated, from 0.015 to 0.059 (as carbon), increased the daily maximum ozone concentration by 12 percent, even though the increase in total carbon was offset by decreases in the amount of aromatic and olefinic compounds. Results in Tulsa show an increase in the fraction of oxygenated organics, from 0.008 to 0.036, has considerably less effect, however, than a reduction of 12 percent in total hydrocarbon emissions. In this test, the net effect

was to lower the daily maximum ozone prediction by 9 percent. About half the reduction in total hydrocarbon emissions was accounted for by aromatic compounds, the other half by paraffins, on a per carbon basis. Taken together, the results from these studies indicate that accurate model predictions require that attention be given to the composition of emitted hydrocarbons and especially to emissions of oxygenated organic compounds.

5.5 Interaction with Emission Reductions

Of special interest is the interaction between emission reductions and uncertainties in other model input parameters. Changes in ozone concentrations which are predicted to occur as emissions are reduced may be influenced significantly by other model inputs. However, very limited analyses have been done in this area. In the Tulsa study, simulations of the effect of a 30 percent reduction in hydrocarbon emissions were made for two different levels of background hydrocarbon concentrations aloft. Background hydrocarbons differed by a factor of two (42 vs. 84 ppb C at 500 meters altitude) while organic oxygenates differed by a factor of three (4 vs. 12 ppb C at 500 m) for the two cases. At the lower background level, the daily maximum ozone was reduced by 27 percent. However, at the higher background level, ozone was reduced only half as much, just 14 percent.

The Denver study examined the effect of vertical mixing on the relative change in ozone concentrations when emissions are increased. A modification was made to the exposure class which corresponds to a change from unstable to neutral stability. The daily maximum ozone prediction was increased nearly twice as much for the neutral case as

for the unstable case. It appears from these results, together with those from Tulsa, that emission control requirements could be quite sensitive to the extent to which urban emissions are dispersed and become mixed with background air.* Thus, the accuracy of estimates of needed emission controls may depend significantly on the availability and reliability of background air quality measurements and on the treatments of winds and vertical mixing, all of which act in complementary fashion.

5.6 Conclusions

Tests of model sensitivity in the four studies allow the following conclusions to be reached. Users are cautioned that these are based on limited sensitivity analyses which cannot be generalized to apply to all situations.

- Background air quality levels for ozone and organic compounds can be expected to significantly influence ozone predictions, particularly when emissions are reduced. Proper characterization of these is needed to better ensure the accuracy of model predictions, particularly the characterization of hydrocarbons and oxygenated organic compounds.

- Vertical mixing of emissions with background air exerts a strong effect on model ozone predictions. Users should realize the extent of mixing depends on a complex interplay involving a number of model input parameters. The specification of these must be coordinated to achieve good results. Given the significance of vertical mixing and the difficulty of representing turbulent diffusion in atmospheric models, independent evaluation of this component of the model is suggested in order to better ensure the accuracy of the model predictions.

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*This is also consistent with the significant difference found in the Denver study with respect to the two versions of the model discussed in Section 2. The version with less "numerical diffusion" gave a relative reduction in the peak ozone which was one third greater, for the same emission reduction.

- Users should be aware that NO_2 photolysis rates have a strongly controlling effect on model ozone predictions. In the present formulation of the model, only a relatively simplistic approach to the specification of the NO_2 photolysis rate is possible. In the interest of greater accuracy a more realistic representation of these rates is needed, one based on physical mechanisms for radiative transfer in urban atmospheres.

- Alternative distributions of hydrocarbon emissions in terms of chemical composition can be expected to produce significant changes in ozone predictions under certain circumstances. These changes are related to differences in the reaction rates and pathways of different hydrocarbon species. Relatively large perturbations are required to produce major effects. However, organic oxygenates appear to have an effect on ozone concentrations which is out of proportion to their relative rate of emission compared to hydrocarbons. This reflects the high degree of efficiency with which these compounds promote ozone formation in the Carbon-Bond Mechanism. Particular attention to these compounds in the preparation of emission inventories appears necessary to improve the accuracy of model predictions.

6. ANALYSIS OF CONTROL STRATEGIES

The studies in all four cities have analyzed the effect of emission controls on model ozone predictions. Specific control strategies, involving emission reductions for individual sources or source types, and uniform emission reductions, involving across-the-board emission reductions for all sources, have both been examined. Since the studies in St. Louis, Denver, and Tulsa were conducted or sponsored by EPA, emphasis is given to the results from these studies. Control strategy work in Los Angeles was done under private auspices and is not included. Control strategy simulations have been performed on three days in St. Louis, two days in Tulsa, and eight days in Denver. Analysis of the results of these simulations has focused on the daily maximum ozone predictions.

6.1 Predicted Effects of Emission Reductions

Control strategy simulations for St. Louis and Tulsa show that for a given reduction in hydrocarbon emissions at constant NO_x, the daily maximum ozone concentration is reduced by a percentage which is less than or equal to the percentage reduction in emissions. The St. Louis and Tulsa results are shown in Figures 13 and 14 in the form of ozone response curves. These give the relative change in the daily maximum ozone prediction versus the relative change in hydrocarbon emissions. Immediately evident is the large disparity in the results from one simulation day

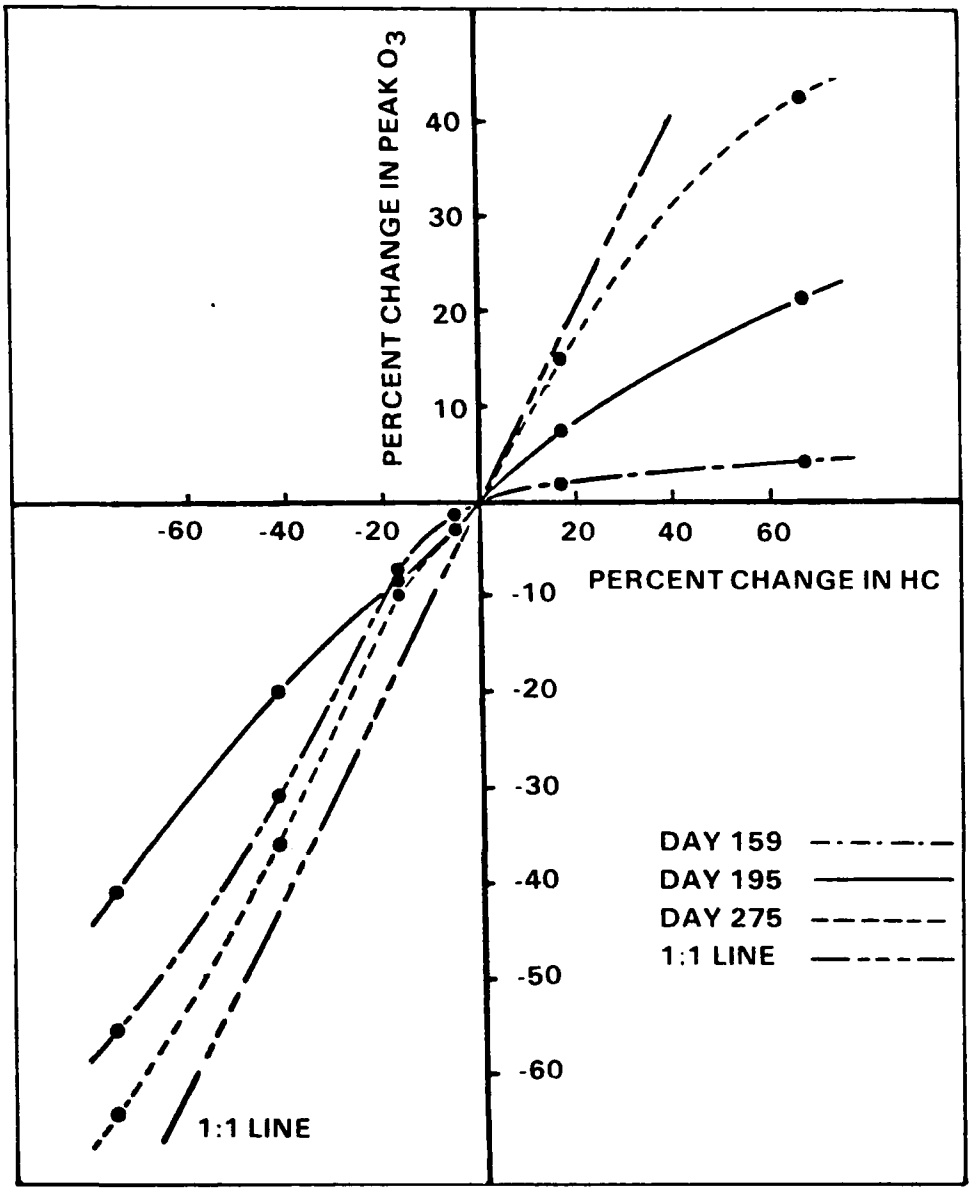

Figure 13. Ozone response curves, St. Louis.

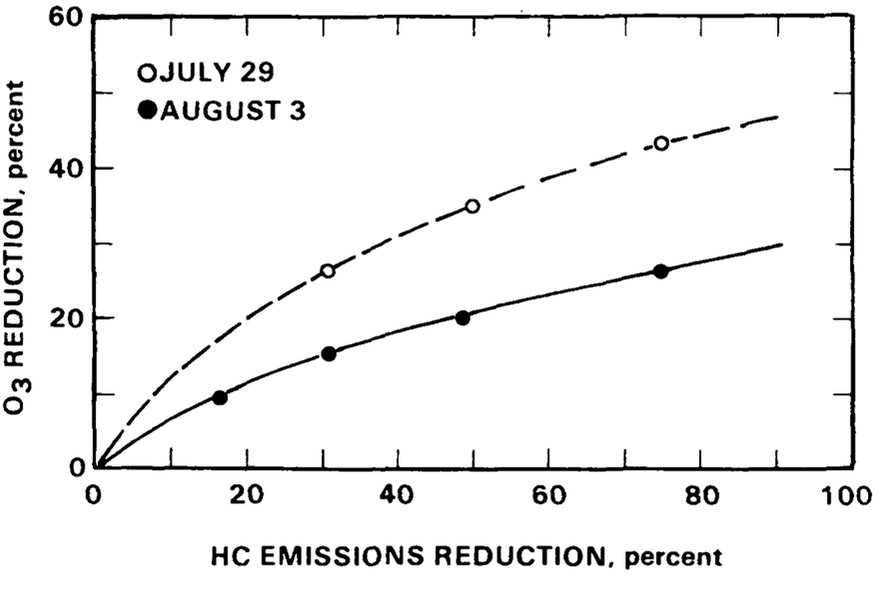

Figure 14. Ozone response curves, Tulsa.

to the next. This is a reflection of the strong dependence which ozone concentrations have on both meteorology and background air quality. The shapes of the curves appear to be somewhat different for the two cities, the Tulsa response curves flattening much faster as hydrocarbons are reduced. However, this merely reflects the lower ozone concentrations which prevail on the Tulsa days. As emissions are reduced, the relative change in ozone is lessened as background levels of ozone and its precursors are approached.

Results from the St. Louis and Tulsa studies suggest there is little relationship between the maximum observed or predicted ozone concentration and the sensitivity of model ozone predictions when emissions are changed. This is illustrated more clearly in the results from the Denver study shown in Figure 15. From this diagram, there appears to be no correlation between the percentage reduction in ozone due to a change in emissions and either the maximum ozone observation or the maximum ozone prediction. Different days exhibit different ozone reductions for the same emission reduction.

A potentially significant finding of the St. Louis study is the tendency of the daily maximum ozone prediction to migrate downwind as hydrocarbon emissions are reduced. This suggests that rather than basing required emission controls on ozone predictions at a particular monitoring site, controls should be based on the daily maximum prediction, regardless of location. Otherwise, the ozone problem may simply be shifted downwind, to locations further from the immediate urbanized areas of the city.

Looking at individual control measures, results for both Tulsa and St. Louis show that controls on mobile source hydrocarbon emissions

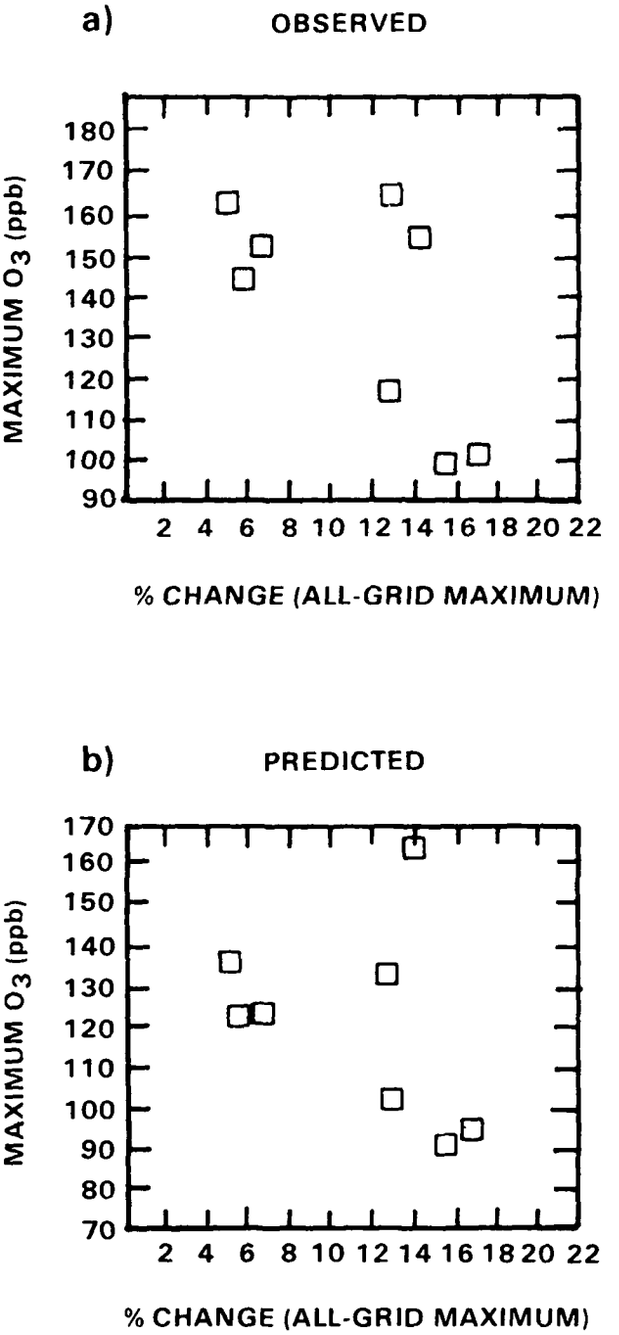

Figure 15. Ozone reduction vs. (a) maximum observed O_3 and (b) maximum predicted O_3 for a change in emissions, Denver. (Adapted from Dennis et al. 1983).

are more effective than controls on stationary source hydrocarbon emissions on a pound-for-pound basis. This is because mobile source emissions have larger olefin, aromatic, and aldehyde components than do stationary sources. These compounds contribute to the formation of ozone with greater efficiency than do paraffins.

The St. Louis simulations also indicate that controls on hydrocarbon emissions from both stationary and mobile sources combined cause ozone to be reduced more than indicated by the sum of the reductions for the two source types individually, as if having a synergistic effect. The synergism is a reflection of the nonlinearity of the ozone response curves. This can be seen from Figure 13, where the curves are shown to be slightly S-shaped when emissions are reduced.

Very little systematic study has been done on the effect of changes in NO_x emissions, either increases or decreases, on daily maximum ozone concentrations. Results from the St. Louis study indicate that decreases in NO_x emissions tend to offset ozone reductions achieved by controlling hydrocarbon emissions. However, studies done in Los Angeles reportedly show the opposite. Ozone formation is limited in part by rapid NO_x removal mechanisms under Los Angeles type conditions. Substantial reductions in both hydrocarbons and NO_x appear to be necessary to cause large reductions in ozone in the eastern part of the Los Angeles basin. A similar effect may occur downwind of other urbanized regions in rural areas. Thus, although increases in NO_x emissions may decrease urban ozone levels, ozone levels in rural areas may be increased. However, the role of urban NO_x emissions in rural ozone formation remains speculative.

6.2 Estimation of Emission Control Requirements

Model simulation results show clearly that ozone formation is a complex process in which emissions, meteorology, and background air quality interact. The day on which the highest ozone concentration is observed is not necessarily the day that will require the greatest emission controls. Results from both the Denver and Tulsa studies suggest ozone reductions may be more difficult to achieve on days when the daily maximum ozone prediction is located in outlying areas, away from the immediate urban environs. Considerations such as these, combined with the fact that the monitoring network may not detect the highest ozone concentrations on any particular day, dictate that several days, at a minimum, be simulated for the purpose of control strategy development.

Ozone response curves, such as those in Figures 13 and 14, are a useful tool for estimating emission control requirements. Given the percentage reduction needed to lower the maximum prediction on a particular day to the level of the standard, the curves provide an estimate of the required percentage reduction in hydrocarbon emissions. In this way, the model results are used in a relative sense. The advantage to this approach is that model errors are implicitly controlled. For example, if the relative error (percent over or underprediction) in the maximum prediction is the same in the pre- and post-control simulations, then the relative change in the maximum ozone prediction will remain free of error. Using the model in an absolute sense, such that the maximum prediction for the post-control scenario is not allowed to exceed the level of the air quality standard, could lead to either an over or

underestimation of the degree of emission control required depending on whether the model is over or underpredicting the maximum concentration.

In many situations, however, the relative error would not be expected to remain constant, in part due to the strong nonlinearity of the model. In addition, the inputs themselves may readily contribute to a nonlinear type of behavior. For example, in a typical control strategy simulation, background concentrations, presumably associated mainly with uncontrolled anthropogenic, biogenic, or other sources, are held constant while emissions are reduced. In this way, uncertainties in the specification of background concentrations can have a large effect on the relative change in the peak ozone prediction in response to emission reductions.

6.3 Veracity of Control Predictions

In studies employing the SAI Urban Airshed Model, and indeed in most air pollution modeling studies, the assumption is made that if it can be demonstrated a model adequately reproduces air quality observations for one emissions level, then the predictions will be equally valid at another, generally lower, emissions level. This may frequently be a reasonable assumption for nonreactive pollutants, but is more likely to be a matter of faith for photochemical pollutants such as ozone. The strongly nonlinear character of atmospheric chemical reactions can nullify such assumptions. Dennis et al. (1983) argue it is necessary to test the veracity of control predictions directly.

An attempt to do this was made in the Denver study. Model simulations for an ensemble of eight days were conducted with emission

inventories for two different historical periods. The average change in the daily maximum ozone prediction was compared to the trend in observed ozone concentrations during an overlapping time period. Although trend analysis is necessarily imprecise, due largely to the confounding effects of meteorology, the results are encouraging. The average change in the daily maximum ozone prediction (10.9%) agrees favorably with the observed trend (13.6% change) despite the fact that the peak ozone concentrations are themselves significantly underpredicted in the Denver study. The reliability of these results is difficult to judge, however, due in part to inconsistencies between observed and predicted trends in nonmethane hydrocarbon and NO_x concentrations. Only by means of ongoing modeling efforts and continuation of monitoring programs, both for ozone and its precursors, will it be possible to demonstrate conclusively that photochemical models are capable of predicting changes in ozone concentrations which occur due to the implementation of emission control strategies.

6.4 Conclusions

Applications of the SAI Urban Airshed Model to date allow the following conclusions to be reached. Users are cautioned that these are based on limited analyses which may not be applicable to every situation in which the model might be applied.

- Uniform changes in hydrocarbon emissions will result in nonlinear changes in peak ozone predictions which are in the same direction. However, the magnitude of the relative change in peak ozone is likely to be less than the relative change in emissions.

- The degree of hydrocarbon emissions reductions needed to lower ozone concentrations to the level of the standard can be expected to vary strongly from day to day. Days with the highest observed peak ozone are not necessarily those needing the greatest emission control. Thus, it is essential that control requirements be based on a sample comprised of a number of days.

- Simultaneous reductions in both hydrocarbon and NO_x emissions are likely to be less effective than hydrocarbon emission reductions alone in controlling peak ozone concentrations in or near urban areas. However, the extent to which urban NO_x emissions may contribute to rural ozone is unknown.

- Reductions in mobile source emissions can be expected to be more effective than equal reductions in stationary source emissions. Thus, consideration of differences in the composition of hydrocarbon emissions among source types is recommended for the purpose of control strategy development.

- In some cases, the daily maximum ozone prediction migrates downwind as emissions are reduced. Thus, emission control requirements should not be based on ozone predictions constrained to a particular monitoring site.

- Reductions in background precursor concentrations which parallel emission reductions can be expected to have a substantial effect on peak ozone concentrations for days with moderate to strong wind speed and a lesser effect on stagnation days. Such reductions cannot be recommended, however, as there can be no assurance that background levels will be favorably influenced by emission control efforts.*

- The accuracy of model predictions of the ambient air impact of emission controls is difficult to ensure, even if the usual model performance evaluation indicates good results. This is related to the strongly nonlinear character of atmospheric chemistry and diffusion. Assurance of good control predictions would require the model to be evaluated with data bases which encompass a change in emissions. Unfortunately, suitable data bases of this sort are only rarely available. In this regard, the Denver study provides preliminary indications which are encouraging, although the data available are inconclusive.

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*Background is to be distinguished from interurban transport of freshly emitted ozone precursors between cities closely situated, as in some parts of the Northeastern U.S. Such transport has not been addressed in the four studies.

7. SUMMARY AND PERSPECTIVES

This report has reviewed recent applications of the SAI Urban Airshed Model involving studies in Tulsa, St. Louis, Denver, and Los Angeles. All four cities are relatively isolated from other urban areas. Thus, interurban transport was not a factor in these studies. Both Los Angeles and St. Louis had extensive data bases available, including air quality and meteorological data. In Denver, only a relatively sparse data set was available, derived nearly entirely from routine monitoring activities. Tulsa was intermediate with respect to data availability. All studies used similar techniques in the development of the emission inventories. Neither the simulation program nor the preprocessor programs were identical in the four studies. These similarities and differences must be considered when attempting to generalize from the study results.

The results of the four studies have been discussed in regard to evaluation of model performance, model sensitivity, and analysis of control strategies. It is hoped that potential users of the SAI Urban Airshed Model may benefit from the experience described here. Clearly, however, the reliability of the model results depends heavily on the amount and quality of the data available for modeling and the ability and experience of those persons who must of necessity make various judgments regarding the data, its interpretation, and its suitability and representativeness

with respect to the requirements of the model. Other users may be more or less successful than the results of these studies would suggest.

Conclusions regarding model performance, model sensitivity, and control strategies are given at the end of each section and will not be repeated here. However, some general impressions to leave with the reader are summarized as follows. One is that the accuracy of the model, in terms of agreement between the model predictions and observed ozone concentrations, is judged to be quite good, with the exception of the Denver study where less data were available. When the peak ozone predictions are compared to the peak ozone observations for the ensemble of days modeled in the four studies, the accuracy of the model predictions is on the order of 30 percent. On any given day, the model is more likely to underpredict than to overpredict. It should be recognized that determining the accuracy of the model in a quantitative sense is not a simple exercise; no single statistic is able to satisfactorily characterize the ability of the model to predict the peak 1-hour ozone concentration used for control strategy analyses. Although the studies do suggest a tendency to underpredict the peak 1-hour ozone concentration, sensitivity analyses indicate the tendency to underpredict is well within uncertainties attributable to the model inputs. This does not mean, of course, that the model inputs are responsible for all errors in the model predictions or that the model cannot be improved.

A second impression is that background concentrations, particularly hydrocarbon and oxygenated organic compounds as well as ozone, exert a considerable influence on the model predictions. Although effects

are seen in the base case, the impact of background concentrations is far greater when emissions are reduced. The implications for control strategy analyses are obvious. The importance of background can be assumed to be further heightened the more the plume of urban emissions becomes mixed with background air. This in turn is controlled by the particular set of meteorological conditions on any given day as well as by peculiarities associated with the grid model itself.

Substantial time and effort have been expended to gain perspective on the use of the SAI Urban Airshed Model as a predictive tool for ozone in urban areas. The four studies reviewed in this report underscore the level of resources necessary to mount an application of the model in a particular locale. At present, a total cost of 50,000 dollars can be expected per day simulated. This includes the cost of analyzing the air quality and meteorological data and preparing it for input to the model. Also included are various preliminary simulations and sensitivity analyses which are necessary on any given day to optimize and refine the modeling approach. Special expertise is required to both exercise the model, in a scientific sense, and execute the model, in an operational sense. The per day cost could be higher depending on the complexity of the meteorological regime, for example if terrain or coastal effects are present, and the manner by which these are treated. Paradoxically, the less data that are available for consideration in modeling, the lower the costs are likely to be. Not included is the cost of preparing a spatially, temporally, and chemically resolved emission inventory or the cost of collecting ambient data. Application of a three-dimensional grid model can place additional, more stringent, informational requirements on the

emissions and ambient data bases than are routinely made at the State and local levels depending, in part, on the perceived needs of a particular application. However, the major costs associated with the collection and maintenance of high quality data bases are borne by other air pollution abatement activities and are not unique to modeling.

Due to resource demands, casual or routine application of the model is not feasible. This must be considered in any regulatory usage of the model. Another impediment to routine usage is the lack of complete documentation with respect to operation of the model and adequate guidance concerning the role and significance of various input parameters.

In addition, there are difficulties in the interpretation of model predictions for setting emission limitations. As pointed out earlier, the day on which the highest ozone concentration is observed at a monitoring site is not necessarily the day that will require the greatest emission controls. This is related not only to the nonlinear behavior which occurs when chemical and physical processes interact in the atmosphere, but also to the limited size of monitoring networks. Thus, it is not possible to pick the day a priori upon which emission control requirements should be based. Given the current form of the ozone NAAQS and assuming sufficient data were available, one would need to model every day in a three-year period in order to be sure of selecting the day upon which emission control requirements should be based. In practice, some subset of days during the three-year period, namely those having relatively high observed ozone levels, would likely suffice. This subset of days is anticipated to include a relatively large number of

days that would require modeling. However, modeling of even a modest number of such days requires the expenditure of considerable resources. Further, it is difficult to establish valid criteria for selecting a few days to be modeled. The predictions of the SAI Urban Airshed Model for a small set of days on which high ozone concentrations have been observed simply do not allow any statistically based finding to be made regarding the probability of a violation. The problems discussed here are posed by all complex models, either physicochemical models, such as the SAI Urban Airshed Model, or complicated Gaussian models, where a large number of sources are involved.

Results from the studies reviewed in this report indicate the SAI Urban Airshed Model is capable of reproducing observed ozone concentrations with an accuracy that is comparable to other numerical models in the field of science and engineering and is frequently better than that obtainable from Gaussian models for other pollutants. However, the ability of the model to adequately predict changes in ozone concentrations brought about by emission reduction programs is still an open question. A long-term ambient monitoring and emissions tracking program is required to settle this issue. As a partial interim step, sensitivity studies could be undertaken with the data bases currently available to examine the uncertainties associated with model predictions of the air quality impact of emission controls.

The SAI Urban Airshed Model appears to be best suited as a long-term planning tool. The model is also useful as a benchmark for comparison with simpler photochemical models or as a tool for the development

of State Implementation Plans where resources and data bases permit. As a planning tool, the model is particularly useful for answering "what if?" type questions. If alternative motor vehicle fuels, such as methanol, come into widespread use in the future, how will ozone concentrations be affected? If assumptions which have been made concerning levels of oxygenated organics aloft are off by a factor of two, how will predictions of the air quality benefit of emission controls be influenced? If available data are unrepresentative of winds aloft, how will estimates of needed emission reductions be modified if an alternative wind treatment is used instead? In order that determining the answers to these questions might be other than an exercise in model sensitivity, devoid of reality, the model must have a firm scientific footing.

In order to serve in these capacities, the model must be accepted as "state of the art" by the air pollution community. Periodic improvements in the formulation of the model to incorporate research developments in the fields of photochemistry and turbulence and diffusion will likely be required if regulatory needs call for the retention of such a role into the future. Areas where such developments may prove fruitful lie with (a) the further refinement of the chemical kinetics mechanism, particularly the chemistry of aromatics and the treatment of background reactivity, (b) the coupling of photolytic rates with atmospheric radiative transfer, (c) the treatment of vertical mixing in the planetary boundary layer, (d) the explicit treatment of sub-grid scale point source diffusion, and (e) the creation of three-dimensional wind fields from sparse data sets.

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16. ABSTRACT

Reviewed are studies in St. Louis, Denver, Los Angeles, and Tulsa on the use of the SAI Urban Airshed Model for the development of strategies for ozone control. The SAI Urban Airshed Model is a three-dimensional photochemical grid model incorporating the Carbon-Bond Kinetics Mechanism. The report discusses the availability of aerometric data in the four studies and the sensitivity of model predictions to selected input parameters. An analysis is presented of the performance of the model with respect to ambient ozone observations. Issues and results pertaining to use of the model for control strategy analyses are identified and discussed. It is anticipated that potential users may benefit from the experiences in applying the model which are described here.

17. KEY WORDS AND DOCUMENT ANALYSIS

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