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Project Summary

1978 Houston Oxidant Modeling Study Volumes I and II

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During the period 15 September through 12 October 1978, the U.S. Environmental Protection Agency (EPA) conducted a special program that monitored air quality and meteorology in the Houston, Texas area. The objectives of the program were to obtain a comprehensive data base suitable for use with photochemical air-quality simulation models and to provide a detailed body of data that can be used to investigate Houston's air quality in general and photochemical oxidants (HOMS Study) and aerosols (HACS Study) in particular.

The objectives of this contract were (a) to evaluate the suitability of the 1978 Houston data base for photochemical modeling application, (b) to analyze spatial and temporal patterns of pollutant concentrations, (c) to archive data in a manner suitable for use with air quality simulation models, (d) to analyze and characterize the quality of the gaseous pollutant measurements, and (e) to use the data to evaluate the performance of the EKMA photochemical model. Results from the data evaluation and archiving work are reported in a three-volume report. (Results from the EKMA evaluation work are reported in a separate report.)

The data evaluation effort is reported in Volumes I and II, summarized here, and the data quality characterization effort is reported in Volume III.

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

Introduction

During the period 15 September to 12 October 1978, the U.S. Environmental Protection Agency (EPA) conducted an intensive program that monitored air quality and meteorology in the Houston, Texas area. The purpose of the program was twofold:

- To obtain a comprehensive, high quality data base suitable for use with photochemical air-quality simulation models.
- To provide a detailed body of aerometric data that can be used to investigate Houston's air quality in general, and photochemical oxidants and aerosols in particular.

In keeping with these objectives, the monitoring program consisted of two complementary parts known respectively as the Houston Oxidant Modeling Study (HOMS) and the Houston Aerosol Characterization Study (HACS). The data collected during the program were subsequently forwarded to SRI, where the measurements were assembled into a unified data base and subjected to various analyses, the results of which are described in this report. Included in this effort is a comparison of the HOMS data to those obtained in previous Houston studies, the most comprehensive of which is the Houston Area Oxidants Study (HAOS) conducted in the summer of 1977. The HAOS aerometric data have been analyzed by SRI investigators, and some of their results will be compared with those obtained in the present investigation.

More specifically, the objectives of this project are:

- To evaluate the suitability of the 1978 Houston data base for use with photochemical air quality simulation models.

- To analyze pollutant concentration and meteorological data.
- To assemble a data base.

The results of this project are reported in two volumes. This volume, Volume I, describes the evaluation and analysis of the data, and Volume II contains a guide to the data base. A companion report will be published later that will examine the quality of the measurements. Also, in accordance with the project's scope of work, a paper describing preliminary results was presented at the Specialty Conference on Ozone/Oxidants sponsored by the Air Pollution Control Association (APCA) that was held in Houston in October 1979. The paper has been included in the conference proceedings published by APCA.

Evaluation of HOMS Data Base

The HOMS monitoring program produced data that describe in detail the spatial and temporal variations of ozone, because the ozone monitoring network was relatively dense. Consequently, there is a rich ozone data base that can be used for testing the ability of photochemical models to predict ozone.

Photochemical models require specification of the initial and boundary concentrations of hydrocarbons and NO_x. In this respect, the HOMS coverage was not as complete as for ozone. The disposition of the monitoring stations left gaps in the southwestern half of the modeling region for both hydrocarbons and NO_x. This can create problems in specifying initial conditions since our analysis, which used empirical orthogonal functions, showed that there are small-scale variations in the spatial patterns of hydrocarbons and NO_x. Since the small-scale changes are not well defined in large areas of the modeling region, the use of interpolation to estimate initial conditions can yield poor approximations of actual concentrations.

Because three-dimensional effects are so important in the formation and transport of ozone, we focused our attention on the 19 days when aircraft data were available. About half were judged to have reasonable good data for defining initial conditions. Data were deemed suitable for specifying boundary conditions at the upwind edge of the region on 13 of these days. Regarding boundary conditions we recommend that future programs include aircraft flights that circumnavigate the modeling region, since this would enhance the model's ability to specify accurate boundary conditions. Several of the HOMS flight paths ranged far from the modeling region, and consequently the data obtained are not very useful for purposes of modeling conditions in the urban area itself.

Aldehydes are an important input in modern photochemical models but they are seldom measured. Total aldehydes and formaldehyde were monitored during the HOMS on a limited basis. Although the data obtained are useful, the amount is insufficient to permit a detailed characterization of temporal and spatial fluctuations. Future monitoring programs should include more extensive efforts to measure aldehydes. Specifically, it would be preferable to measure aldehydes for an extended period at a few well-chosen locations than to monitor for short periods at several sites, as was done in the HOMS.

The 0600-0900 (CDT) NMHC/NO_x ratio is an important descriptor of ozone-precursor conditions. Both NMHC and NO_x were measured concurrently at only six of the monitoring sites and the data capture rate at four of the sites was rather low, so the ratio could be estimated for only 30 of the maximum possible 108 site-days at those four sites. The two remaining sites had a combined data capture rate of 45 of a possible 54 site-days. Thus, the analysis of patterns of NMHC/NO_x ratios in the HOMS is limited by the relatively small amount of data. Incidentally, the HAOS data are similarly afflicted, having captured about 26 percent of the possible NMHC/NO_x ratios at five sites.

The number of monitoring sites where meteorological parameters were measured varied between one and five during the 19 days of aircraft operations. Such coverage is very sparse, and may be inadequate for modeling applications. To compensate for the sparseness of the meteorological data, mass-conserving interpolation methods should be used to generate the wind field that is an input of photochemical air-quality models. **The need for a good wind-field generator for modeling studies is also suggested by the case studies of particular days. These show that wind-shear effects can be important determinants of ozone levels. Although current models treat such effects, they can do so only if the proper wind inputs are provided.**

The HOMS coincided with a period when the Houston area recorded some of its highest ozone levels ever. This is fortunate in the sense that the air quality data can be used to model worst-case or near-worst-case conditions, which of course are of interest for regulatory reasons.

Despite the high ozone levels, both PAN and NO_2 concentrations were relatively low, a result that confirms the findings previously reported for the HAOS. Th HOMS analysis showed that the highe NO_2 levels occurred in downtow Houston and in locations west and nortl west of downtown. PAN was measured one rural location (Sheldon, Site 18) ar one suburban site (Jackrabbit, Site 2C Mean PAN values do not differ very muc at these two sites, but the maximum PA at Jackrabbit is more than twice that Sheldon.

Detailed hydrocarbon analyses wer conducted at 10 sites located in industria urban, suburban, and rural areas. Th analysis of 11 selected compounds for th period 0800-0900 showed that ethan and propane are relatively uniformly dis tributed. Acetylene and propylene cor centrations have similar, nonuniform spa tial distributions. Isopentane and isobu tane exhibit considerable spatial fluctua tions, as do toluene and the xylenes Benzene shows a dichotomous spatia pattern: industrial, urban, and suburba sites have similar mean concentration that are significantly higher than for site on the fringes of the urban envelope. N butane follows a comparable pattern, ex cept that the industrial site clusters wit the outlying locations.

Mobile sources were found to be re sponsible for acetylene and propylene a several locations, including downtow Houston, which was expected. Howeve evidence of stationary sources contribute by propylene was also found at a numbe of sites. Benzene was found to follow th same pattern as propylene. At all the site examined, toluene and the xylenes ap peared to receive substantial contribu tions from stationary sources. The same i true for isopentane and the two butanes

The HOMS and HAOS hydrocarbon dat were compared and found to be generall consistent in the pattern of concentration and hydrocarbon/acetylene ratios. How ever, the benzene/toluene ratio in th HOMS data was different from that in th HAOS measurements. The indications ar that the benzene/toluene ratio in th HAOS may not be correct.

The 0600-0900 detailed hydrocarbo data for the HOMS were compared wit similar data from Denver and southern California. Denver's hydrocarbon mixtur was found to be similar to that in suburba Houston. The mixtures in downtown Hous ton and Los Angeles were also found to b similar except for toluene and the xylenes for which levels in the Los Angeles are were considerably higher than in Houston In general, the southern California dat differ most markedly from Houston's the higher content of aromatics, whic

appear to be mainly due to stationary sources.

The 0600-0900 n-butane/propylene ratio is used as an indicator of the reactivity of the hydrocarbon mixture in some air-quality models. For this reason, we compared these ratios in Houston, Denver, and southern California. The mean and median ratios at four of five sites in southern California were somewhat lower than in Houston or Denver, which suggests that the mixture may be slightly more reactive. In particular, the ratio in downtown Houston is higher than in downtown Los Angeles, but is similar to the ratio at Long Beach.

The analysis of the aldehyde data showed that formaldehyde ranged from 1 to 28 ppb, and total aldehydes from 4 to 40 ppb. The highest aldehyde levels were associated with elevated ozone concentrations. However, although formaldehyde exceeded 20 ppb only when maximum daily ozone was at least 100 ppb, the converse is not generally true.

Examination of 0600-0900 (CDT) NMHC/NO_x ratio showed that they ranged from 1 to 210, with six ratios having values exceeding 100. Ninety-two percent of the ratios did not exceed 85. The median ratio for the area was 14, which is similar to the median ratio of 12 found in the HAOS. The distributions of the HOMS and HAOS ratios were compared and found to diverge substantially at the high end. The divergence is caused by the presence of several very high values in the HOMS data, ratios that are high because the NO_x was very low, not because NMHC was high.

The spatial patterns of NMHC, NO_x, and ozone were analyzed using empirical orthogonal functions. The analysis showed that the spatial distribution of ozone has a high degree of uniformity, and is characterized by large-scale features. By contrast, the spatial distributions of NMHC and NO_x are less uniform and show evidence of small-scale influences. These results imply that the ozone-monitoring network need not be as dense as it was, but that the number of stations monitoring NMHC and NO_x probably should be more numerous to capture the small-scale features. For NMHC and NO_x, these results imply that it may be inaccurate to estimate initial conditions for a grid-type model by interpolation or extrapolation based on the monitoring network.

Several days were identified that may be of interest for modeling applications. An ozone episode occurring from 1 through 5 October 1978 seemed particularly interesting. Case studies of potential modeling days were performed for 20 and 29 September and 1 and 2 October. The case studies showed the influence of conditions aloft on ground-level concentrations. It is clear from these and other studies that the processes affecting the formation and transport of ozone are very three-dimensional. Thus, if modeling efforts are to succeed, it is important that the models be provided with accurate well-resolved initial and boundary conditions. Moreover, the performance of the models should be evaluated at both the ground-level stations and at points aloft for which measurements exist.

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***K. Demerjian** and **B. Dimitriades** are the EPA Project Officers (see below).*
This Project Summary covers Volumes I and II of three volumes of the complete report, entitled "1978 Houston Oxidant Modeling Study."
"Volume I. Data Evaluation and Analysis," (Order No. PB 83-194 191; Cost: $14.50, subject to change)
"Volume II. Data-Base Guide," (Order No. PB 83-194 209; Cost: $11.50, subject to change)
The above reports are available only from:
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