

One area of validation that has not been researched, and should be, is the representativeness of the air quality measuring stations. The air quality stations measure the air from one point, but the model averages the concentrations over an area of 10.4 km² (4 mile²). There is no evidence that values from the station are representative of the cells or of the surrounding area. Some of the stations are located on sites where the local vehicular traffic may have a significant influence on the recorded concentrations; therefore, the concentrations may not be representative of the modeling cell.

The costs of running the model on the Lawrence Berkeley Laboratory computer vary considerably, depending on the priority the run is given. For example, a 24-h run at a priority 10 (highest priority range) costs about \$3500. On the other hand, the same run at priority 3 (lowest range) would cost \$800. Costs also vary considerably, depending on the number of cells in the model.

The most valuable expertise to have in running the models is a knowledge of computers. The Systems Applications, Inc., model has a number of preliminary data preparation programs in addition to APSP and when glitches occur (which is not uncommon), knowledge of computers, computer systems, and computer programming is invaluable.

OUTPUT ANALYSIS

The printed output for the Systems Applications, Inc., model is quite voluminous—24 h of simulation yield about 1200 pages of computer printout. The only practical way to analyze the output, therefore, was to have the output read onto magnetic tape and write computer programs against this file. The output file was, therefore, put into the state computer system and these programs were written. Three principal programs are now available to compare the output of different scenarios. All are printed out by the computer on standard sheets and displayed by gridded cell array over the entire modeling region. These programs produce

1. The maximum concentration of O₃ and the hour it occurred.
2. A grid array that is shaded by using a different symbol for each concentration range. The symbol is progressively darker as the step ranges increase. There is an array for each hour. Thus, the overall impact can be seen qualitatively at a glance.

3. Changes in maximum concentration from the base scenario. This is done by printing the numbers 1 through 9 if the concentrations go up and the letters A through I if the concentrations go down. No change would be a 0. All 9s and I's require examination to see if the change is greater than 9.

The above data displays are useful in assessing a particular strategy's effect on maximum concentrations. They do not give an easily understandable evaluation of the overall impact, either regionally or subregionally. This can be done by developing an index by which the various plans and strategies can be compared. Comparison of hourly concentrations of oxidant for different emissions scenarios for approximately 2500 grid cells is impossible. A powerful approach, then, would be a people-concentration index for the total region and for critical subregions. This index can be obtained by the use of a program that multiplies the population residing in a cell and the sum of all the hourly concentrations in the cell. This product is then divided by the number of hours of simulation to normalize the index. The individual cell indexes can then be aggregated by subregion or the entire region, as desired. This programming is not yet completed. The ability to analyze rapidly the immense amount of output numbers makes computer programming capability a necessity.

AVOIDANCE OF MAJOR PROBLEMS

The following suggestions are for those about to undertake air quality modeling. They may help avoid some of the pitfalls that were experienced by Caltrans.

1. Buy only a modularized model that can be altered easily to keep up with the changes in the state of the art;
2. Have in-house computer expertise available;
3. Insist on a user's manual that gives complete step-by-step procedures on exactly how to operate the model;
4. Know from the beginning what size matrix is needed. If the matrix is too large, it will cost more to run the model and to collect the input data; and if it is too small, the required answers will not be available. Also, carefully examine the correspondence between the model grid and data source grids;
5. Edit all input data carefully; and
6. Be prepared for unforeseen problems.

Oxidant Model Applications: Denver

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In the Denver air quality control region, the abundance of sunlight, the high altitude, and the large per capita automobile population have resulted in a serious oxidant pollutant problem. Local officials have required and the public has supported the use of the latest state of the art to analyze existing air quality and to determine what may be expected in the future. The photochemical oxidant model developed by Systems Applications, Inc., has been used to assess local conditions. The model was calibrated in the winter for a bad carbon monoxide condition and in the summer for a bad ozone condition. The 120 h of carbon monoxide data sets used to compare the measured versus model-predicted values resulted in a correlation coefficient of 0.71. Ozone data for 74 h

resulted in a correlation coefficient of 0.80. Linear regression equations were used to adjust the model for minor unaccountable error for each pollutant. To date, the model has been used to analyze regional air quality situations given various transportation and land use scenarios. This use includes the assessment of air quality control strategies, transportation system alternatives, and alternative routing of a major freeway proposal. Recent innovations in the model have improved chemistry reaction rates; the model output now approaches the precision of pollutant monitoring equipment. The improved model has been used to analyze various land use strategies and will be incorporated into the transportation planning process.

The Federal-Aid Highway Act of 1970, section 109j; of Title 23, U.S. Code, requires that each state evaluate its transportation plans and programs annually as to their consistency with the state implementation plan. Also, environmental impact statements for major highway construction projects often require an in-depth air quality analysis.

AIR QUALITY IN DENVER

Denver's serious air quality situation can be related directly to large-scale automobile usage, restrictive meteorology (such as frequent temperature inversions and low wind speed), and high altitude factors. Denver's air pollution problem is dichotomous, depending on the annual season. The two major pollutants are carbon monoxide (CO) and ozone (O₃). CO is produced by automobile exhausts, and O₃ is the indirect product of the combination of automobile exhausts and sunlight. Short-term exposure to both pollutants has been associated with deleterious health effects.

CO has a double-peaked diurnal pattern that reflects the rush-hour traffic. The highest concentrations of CO occur in the winter months, indicating the strong relationship between the meteorological parameters of wind speed and inversion height and CO. CO is not only a local pollutant; it has a regional character that has been particularly noticeable in major suburban activity centers. The continuous air monitoring project (CAMP) station in downtown Denver has proved to be a good indicator of the CO situation in the Denver Air Quality Control Region (DAQCR); because the area traffic counts are higher at the CAMP station than at other locations in the DAQCR, the CO pollutant concentrations might also be higher.

O₃, on the other hand, has a single-peaked diurnal pattern that reflects the intensity of sunlight. O₃ is related more to solar intensity than to other meteorological parameters; therefore, the highest annual concentrations of O₃ occur in the summer months. O₃ is a major regional pollutant that primarily affects areas in the DAQCR in which people reside rather than areas in which people work. The CAMP station has been a very poor indicator of the O₃ situation in the DAQCR, because it underestimates the problem for the suburban areas.

The pollutants are not bound by city or county limits and may reach episode levels over much of the metropolitan region during periods of severe atmospheric stagnation. The DAQCR has a priority 1 classification for CO and O₃ because in Denver these pollutants often exceed the national ambient air quality standards (NAAQS).

MODEL SELECTION

The condition of Denver's air quality prompted public officials to recommend the use of the latest state of the art in assessing present and future conditions. The Federal Highway Administration (FHWA), the U.S. Environmental Protection Agency (EPA), the state air pollution control commission, and the state department of highways worked together to determine the most appropriate model for the Denver metropolitan area.

Nonreactive regional air quality simulation models were used prior to 1975 to assess CO concentrations. The extent of O₃ pollution prompted a search for a photochemical oxidant model that could predict this pollutant in addition to predicting the nonreactive pollutant, CO. Recent work by Systems Applications, Inc., in the Los Angeles basin prompted the state of Colorado to contact them regarding the use of their air quality simulation model in Denver. Representatives of Systems Applica-

tions, Inc., were encouraged by the availability of data in the Denver area (including traffic assignment on the metropolitan transportation network, automotive emission factors, an inventory of stationary source emissions, a fairly comprehensive network of surface meteorological data, and a limited amount of upper level meteorological data); however, reaction rates of air pollutant species at Denver's high altitude were not known. The reaction rates used in the Los Angeles basin were later adjusted and found to fit local conditions.

Characteristics and prospective benefits derived from the Systems Applications, Inc., model were presented to local EPA, FHWA, and air pollution control district (APCD) officials for their review. Endorsement was obtained and the recommendation was made to use the model for the section 109j air quality assessment statement (1), air quality maintenance plan statement (2), and an environmental impact statement on a proposed Beltway Interstate project (I-470) (3). The model was useful in assessing future air quality, especially when the Denver area's projected rate of growth was considered.

The Systems Applications, Inc., airshed model (4) is based on the numerical solution of the coupled, time-dependent mass conservation equations, expressed as

$$\begin{aligned} (\partial c_i / \partial t) + (\partial u c_i / \partial x) + (\partial v c_i / \partial y) + (\partial w c_i / \partial z) \\ = (\partial / \partial x) [K_H (\partial c_i / \partial x)] + (\partial / \partial y) [K_H (\partial c_i / \partial y)] \\ + (\partial / \partial z) [K_V (\partial c_i / \partial z)] + R_i + S_i \end{aligned} \quad (1)$$

where

∂ = standard mathematical symbol for partial derivative;

x, y, z = location of a point in space on a rectangular coordinate system consisting of three mutually perpendicular planes;

c_i = concentration of species i ;

u, v, w = wind components in the x, y , and z directions respectively;

K_H, K_V = horizontal and vertical turbulent diffusivities;

R_i = rate of production of species i through chemical reaction;

S_i = rate of production of species i from source emissions; and

t = time.

The equations are three-dimensional in order to handle wind convergence and divergence and elevated inversion behavior. In full photochemical applications, up to six chemical species are considered, including reactive hydrocarbons, nonreactive hydrocarbons, NO, NO₂, O₃, and CO. The chemical reaction rate expressions (R_i) are determined from a 15-step kinetic mechanism, and the source term includes emissions from elevated point sources, such as power plants. Emissions from motor vehicles, fixed sources, and other ground-level sources are input to the model through the boundary conditions.

The major components of the model are as follows:

1. Emissions—An emissions inventory must be prepared for all chemical species of interest. This involves calculations of the total mass of pollutants emitted from automobiles, aircraft, and fixed sources into each ground-level grid cell and the mass of contaminants emitted by elevated point sources into grid cells aloft.

2. Meteorology—Meteorological inputs of wind speed, wind direction, and mixing depth must be specified at the centers of all grid cells.

3. Chemical kinetic mechanism—A chemical kinetic mechanism is required if any of the species of interest react in the atmosphere. The mechanism is used to determine the rate at which pollutant concentrations change as a result of chemical reaction.

The nonlinear, coupled partial differential equations that express the conservation of mass of each pollutant comprise the governing equations of the model. Individual reaction rate expressions (from the kinetic mechanism) are incorporated into the equations, and emissions and meteorological data are inputs to the model. The solution is obtained by numerically integrating the governing equations on a three-dimensional grid; the modeling region is overlaid to obtain the temporal variation of pollutant concentrations in each cell of the grid.

The Systems Applications, Inc., model is embodied in seven computer programs. The most important of these is the atmospheric pollution simulation program (APSP), which is used to predict concentrations of air contaminants in the grid cells that comprise the region to be modeled. The other models are specialized data preparation programs that are used to process the large volume of emissions, meteorological, and air quality data employed by APSP. Ground-level emissions from automobiles, aircraft, and fixed sources are combined by the emission program, SAIEMIS, and the emissions data preparation program (EDPP) to produce an array of total pollutant fluxes into each ground-level grid cell. These fluxes are then placed in the emissions data file (EDF). Hourly wind and mixing depth maps are prepared from available wind measurements and inversion soundings through the use of interpolation procedures in the WIND, DEPTH2, and meteorological data preparation programs (MDPP). The output is stored in the meteorological data file (MDF) for subsequent use by APSP. Initial concentrations required in the solution of the governing equations are computed from available air quality measurements in the program, QUAL, and are stored in the initial conditions data file (ICDF). Figure 1 summarizes the overall structure of the airshed simulation package and indicates the flow of information to and from each program.

After the three input data files are created, operating parameters, elevated point source emissions, and chemical kinetics data for APSP are specified and placed on punched cards. APSP is then used to perform the airshed simulation. Pollutant concentrations are predicted for each grid cell. Based on these values, an estimate can be obtained of the predicted contaminant level at each air quality monitoring station or other point of interest selected by the user. The results of the simulation are presented in three forms:

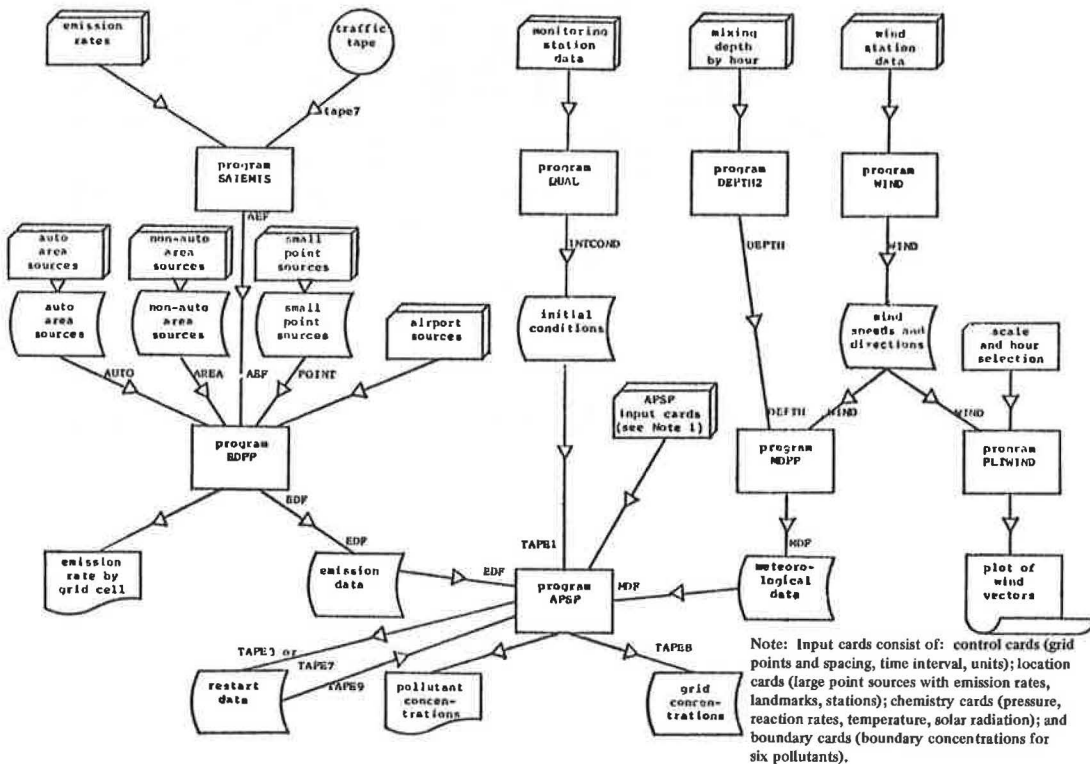
1. Instantaneous ground-level concentration maps for all species, printed at regular time intervals,
2. Printed hourly averaged ground-level concentration maps for all species, and
3. A permanent file containing the instantaneous pollutant concentrations present at the end of the simulation and a permanent file record of all printed output.

Model Calibration

The model must be calibrated for the Denver area to make fine adjustments that cannot be made by using input parameters. This is accomplished by using 2 d to determine the best relation between the measured and predicted values. Extensive monitoring is performed during the 2 d to establish a base. Once the model has been calibrated for current conditions, these factors are used to correct the predicted data for future simulations. These calibrations were based on the emission parameters, which were based on average vehicle route speeds and those emission inputs that incorporated the effect of rush-hour speeds.

The 2 d used to calibrate the model for Denver were November 15, 1974, and July 29, 1975. November 15 was used to observe the ability of the model to predict concentration of CO. July 29 was used to check the

Figure 1. Systems Applications, Inc., model operation flow chart.



ability of the model to predict concentrations of NO, NO₂, hydrocarbons, and O₃.

Figure 2 shows the sites selected for continuous monitoring (in addition to health department permanent stations) of all pollutants used in the model calibration. During the winter calibration for CO, additional sites were selected to determine the nonreactive pollutant concentration by incorporating mylar bag grab samples. Surface meteorological data were obtained from 17 surface sites and upper air radiosonde measurements were obtained from 3 sites. Traffic counters were placed at strategic sites throughout the metropolitan area to obtain a distribution control on the various roadway classifications and area types. The control statistics were later used to adjust annual average roadway link assignments. The conversion was made to obtain hourly traffic distributions on the study day.

The data collected on November 15, 1974, indicated that Denver was under the influence of a temperature inversion from the previous day's frontal passage and accompanying snowfall. This resulted in high CO readings, which were used to calibrate the model for a typical bad winter day. The highest hourly average CO concentration at the CAMP station was 21 mg/m³ (18 ppm), the

117th highest hourly average concentration for the year. The 8-h average for that day, 15 mg/m³ (13 ppm), was the 31st highest 8-h average recorded in 1974. Figures 3 and 4 show the distribution of maximum CO concentrations in Denver. Figures were calibrated in parts per million. Note that 1 mg/m³ of CO = 0.87 ppm.

On July 29, 1975, a maximum O₃ concentration of 0.204 mg/m³ (0.104 ppm) ranked it the 22nd highest hourly average concentration for the year. Figure 5 contains a distribution of 1975 O₃ readings exceeding that value. Note that 1 mg/m³ of O₃ = 0.051 × 10³ ppm. A tabulation of input data except emissions for the model is listed in Table 1. Hourly correction factors for two photo-dependent reaction rates are listed in the second column. These factors rates are listed in the second column. These factors are directly related to the intensity of the sun. Table 2 gives reaction rates for each equation.

The model correlated very well for both days. Figures 6 through 9 are typical plots of predicted and measured concentrations versus time of day. Predicted and measured concentrations were compared using the BMD02R regression program. For November 15, 1974, 120 CO concentrations were compared and had a corre-

Figure 2. Map of Denver metropolitan area.

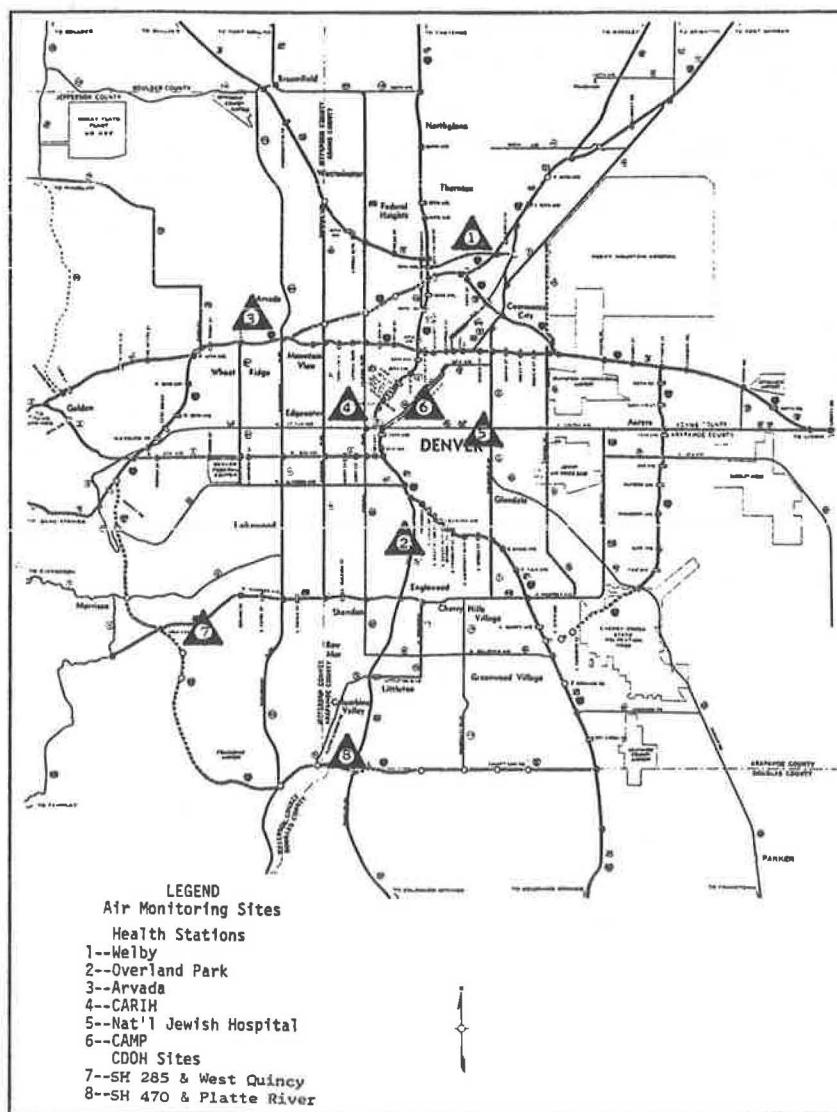


Figure 3. CO concentration exceeding 18 ppm measured on November 15, 1974 at Camp Station.

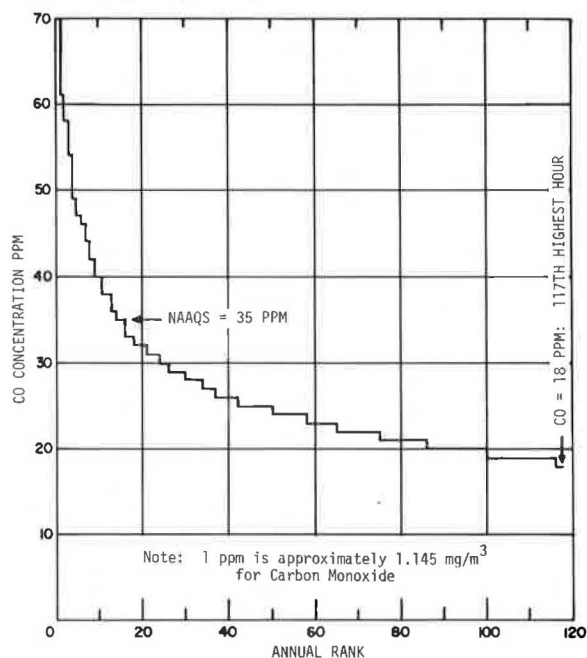


Figure 4. 8-h CO concentration exceeding 13 ppm measured on November 15, 1974 at Camp Station.

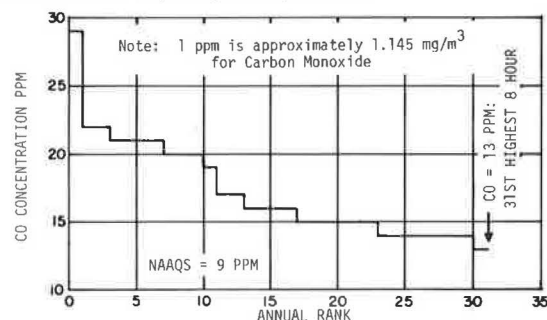


Figure 5. O₃ concentration exceeding 0.104 ppm measured on July 29, 1975 at Overland Station.

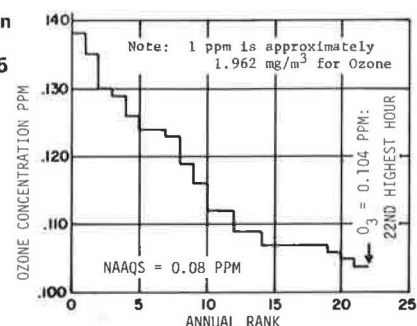


Table 1. Environmental inputs to the Systems Applications, Inc. model for Denver.

Date/Time	Hourly Factor for Reaction Rates	Temperature (°C)	Wind Direction (average)	Wind Speed (average) (m/s)	Inversion Height (m)	Stability Class	Factors for Converting Annual Average Daily Traffic to Hourly Traffic
November 15, 1974							
1:00 a.m.	0.001	-3	SW	1	50	4	0.012
2:00 a.m.	0.001	-2	SW	1	50	4	0.006
3:00 a.m.	0.001	-2	SSW	1	50	4	0.005
4:00 a.m.	0.001	-2	SSW	1	50	4	0.004
5:00 a.m.	0.001	-3	SSW	1	30	4	0.005
6:00 a.m.	0.001	-3	SSW	1	30	4	0.013
7:00 a.m.	0.001	-3	SW	2	30	4	0.049
8:00 a.m.	0.015	-2	WSW	2	75	3	0.105
9:00 a.m.	0.263	0	W	2	150	3	0.076
10:00 a.m.	0.538	2	SSE	2	220	3	0.057
11:00 a.m.	0.677	4	SE	3	350	3	0.052
12:00 noon	0.752	6	SE	3	400	2	0.054
1:00 p.m.	0.752	6	SE	3	400	2	0.053
2:00 p.m.	0.752	6	E	3	435	2	0.058
3:00 p.m.	0.549	7	N	2	500	3	0.064
4:00 p.m.	0.282	5	N	2	375	3	0.078
5:00 p.m.	0.041	4	N	3	150	3	0.101
6:00 p.m.	0.001	3	NW	2	100	4	0.090
7:00 p.m.	0.001	2	W	2	75	4	0.058
8:00 p.m.	0.001	1	WSW	2	50	4	0.038
9:00 p.m.	0.001	1	SW	2	50	4	0.030
10:00 p.m.	0.001	-1	SW	1	50	4	0.030
11:00 p.m.	0.001	-1	SW	1	50	4	0.027
12:00 midnight	0.001	-2	SW	1	50	4	0.020
July 29, 1975							
1:00 a.m.	0.001	20	SSW	2	60	5	0.005
2:00 a.m.	0.001	19	S	1	50	5	0.004
3:00 a.m.	0.001	18	S	1	50	5	0.003
4:00 a.m.	0.001	18	S	1	50	5	0.004
5:00 a.m.	0.001	17	S	1	50	5	0.013
6:00 a.m.	0.19	19	SSE	1	50	5	0.047
7:00 a.m.	0.69	21	SSE	1	100	2	0.085
8:00 a.m.	1.06	24	SSE	2	260	2	0.052
9:00 a.m.	1.39	26	SE	2	350	2	0.048
10:00 a.m.	1.60	27	ENE	3	420	3	0.045
11:00 a.m.	1.60	29	NE	3	940	3	0.049
12:00 noon	1.60	31	E	3	2000	2	0.048
1:00 p.m.	1.60	31	N	3	2000	2	0.051
2:00 p.m.	1.42	33	NNW	3	3260	2	0.059
3:00 p.m.	1.12	33	NW	4	2570	3	0.065
4:00 p.m.	0.78	33	WNW	3	2570	3	0.089
5:00 p.m.	0.27	30	WSW	3	250	3	0.068
6:00 p.m.	0.001	29	SW	4	240	4	0.048
7:00 p.m.	0.001	27	SW	4	200	4	0.050
8:00 p.m.	0.001	22	SW	4	160	4	0.039
9:00 p.m.	0.001	23	SW	4	130	5	0.036
10:00 p.m.	0.001	21	SSW	3	50	5	0.039
11:00 p.m.	0.001	21	SSW	3	50	4	0.043
12:00 midnight	0.001	21	SSW	2	50	4	0.010

Notes: °C = (°F - 32)/1.8, 1 m = 3.3 ft, and 1 m/s = 3.28 ft/s.

The Systems Applications, Inc. model uses 17 wind recording stations to establish a wind pattern.

lation coefficient of 0.712 and a linear regression equation of

Measured value = $0.6 \times$ predicted concentration, using average vehicle speeds

(2)

Table 2. Reaction rates for Systems Applications, Inc., model.

Equation ^a	Rate	
	November 15, 1974	July 29, 1975
1	0.266	0.44
2	3 540 000	2 760 000
3	16.2	21.8
4	0.002 6	0.006
5	0.1	0.1
6	0.000 5	0.000 5
7	0.003	0.008 9
8	176	200
9	1 599	1 800
10	3.88	10
11	5 105	7 278.75
12	3 683	9 486.25
13	0.001 66	0.001 87
14	1 800	1 800
15	13.8	13.787 5

^aEquations can be found in the Systems Applications, Inc., manual (4).

These statistics were later refined by adjusting vehicle speeds to compensate for rush-hour congestion.

On July 29, 1975, 74 O₃ concentrations were compared and had a correlation coefficient of 0.80 and a linear regression equation of ($1 \text{ mg/m}^3 = 0.051 \times 10^3 \text{ ppm}$):

$$\text{Measured value} = 0.95 \times \text{predicted concentration} + 0.053 \text{ mg/m}^3 \quad (3)$$

The regression equations and correlation coefficients for the pollutants predicted may be found in Table 3. These calibrations were then incorporated into the model output to obtain concentrations for the given study day.

Application of Model

Emissions from automobiles, aircraft, and fixed sources are combined to produce an array of total pollutant fluxes into each 2.6-km^2 (1-mile^2) ground-level grid cell contained in the $48.3 \times 48.3\text{-km}$ ($30 \times 30\text{-mile}$) Denver metropolitan area. Hourly wind and mixing depth maps are then prepared from available wind measurements and inversion soundings for each grid cell through the use of interpolation procedures. Model outputs for surface meteorological conditions are displayed in Figures 10 through 12. The actual airshed simulation uses the

Figure 6. CO concentrations: Overland Station, Nov. 15, 1974.

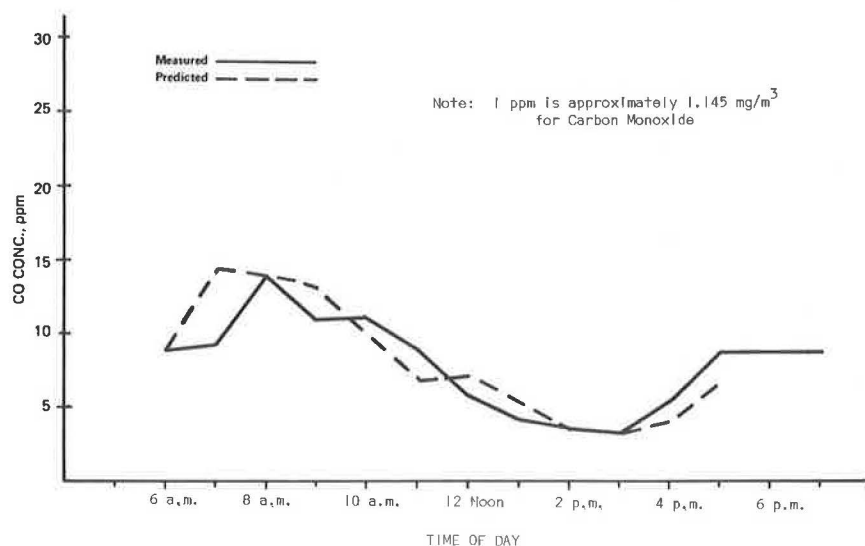
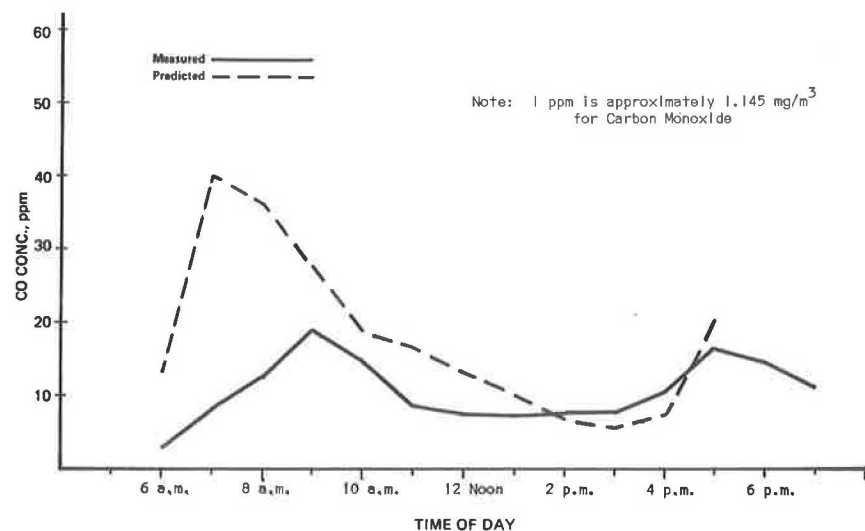


Figure 7. CO concentrations: Camp Station 6, Nov. 15, 1974.



emissions and meteorology to yield the spatial and temporal distribution of contaminants throughout the model region.

The output from the transportation modeling process is used for automotive emissions. This output consists of a highway system that includes a trip table. Each link in the highway system has an assigned traffic volume based on the number of trips desiring to use the link. These link volumes were multiplied by appropriate emis-

sion factors and assigned to their respective grid cell for direct input into the airshed model. The traffic assignments that were used depended on the transportation alternative being tested and the study year.

Emissions, both mobile and stationary, were the only parameters changed when executing the model simulation. Hence, the output was labeled for a given transportation system and a given year on the study day (November 15 for CO and July 29 for O₃).

In order to determine to what extent the standards would be exceeded during the year being studied, a relation between the second maximum concentration measured during the calibration year and the concentration measured on the calibration study day was determined. This relation factor was then applied to the study day for projected years. Typical output distributions of pollutants are found in Figures 13 through 15 (1). Similar displays appear in the air quality maintenance planning (AQMP) study for air pollution control strategies and the I-470 environmental impact statement (2) for various project alternatives. A quantitative system for ranking alternatives was also included in the I-470 statement. This technique used the probabilities from the normal distribution curve to compute violations of the standard and thereby allow for the inaccuracy of the model.

Table 3. Systems Applications, Inc., model calibration used in Denver.

Condition	Pollutant	Measured Value	Standard Deviation
Average vehicle speed	CO	$0.6 \times PV$	4.8
	O ₃	$1.26 \times PV$	0.057
	THC	$1.20 \times PV$	0.33
	RHC	$0.43 \times PV$	0.22
	URHC	$0.95 \times PV$	0.18
	NO	$0.34 \times PV$	0.069
Peak/off-peak vehicle speed	NO ₂	$0.97 \times PV$	0.047
	CO	$0.75 \times PV$	3.8
	O ₃	$(0.95 \times PV) + 0.053 \text{ mg/m}^3$	0.033
	THC	$(0.44 \times PV) + 0.72 \text{ mg/m}^3$	0.34
	RHC	$(0.30 \times PV) + 0.21 \text{ mg/m}^3$	0.121
	URHC	$(0.44 \times PV) + 0.64 \text{ mg/m}^3$	0.073
	NO	$(0.20 \times PV) + 0.05 \text{ mg/m}^3$	0.055
	NO ₂	$(0.66 \times PV) + 0.04 \text{ mg/m}^3$	0.041

Note: For CO, $1 \text{ mg/m}^3 = 0.87 \text{ ppm}$; for O₃, $1 \text{ mg/m}^3 = 0.051 \times 10^{-3} \text{ ppm}$; for NO, $1 \text{ mg/m}^3 = 0.081 \times 10^{-3} \text{ ppm}$; for NO₂, $1 \text{ mg/m}^3 = 0.053 \times 10^{-3} \text{ ppm}$; for HC, $1 \text{ mg/m}^3 = 0.153 \times 10^{-3} \text{ ppm}$; and PV = the predicted value.

Figure 8. O₃ concentrations: Overland station, July 29, 1975.

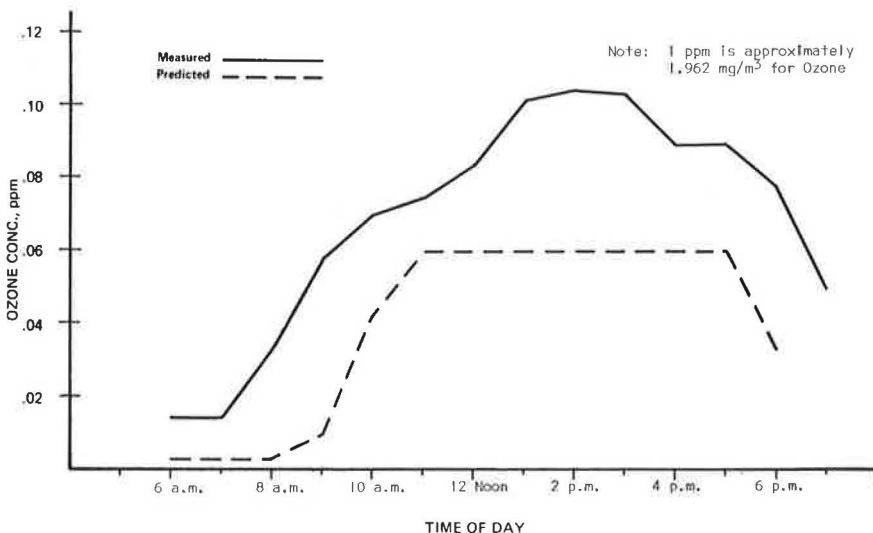


Figure 9. O₃ concentrations: Camp station 6, July 29, 1975.

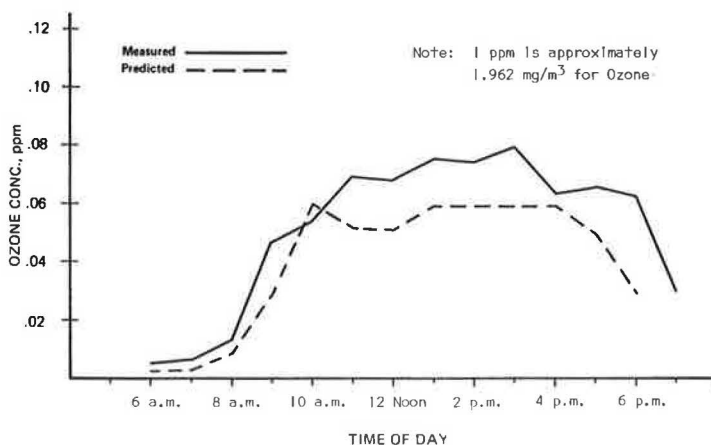


Figure 10. Systems Applications, Inc.,
model-generated surface winds at 5:00 a.m.
MST, July 29, 1975.

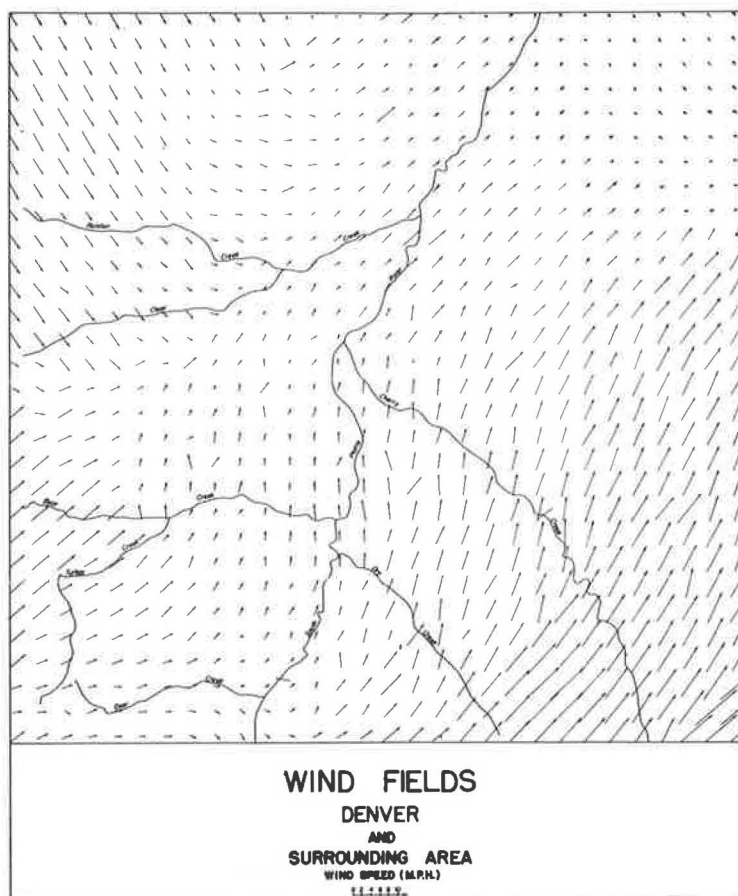


Figure 11. Systems Applications, Inc.,
model-generated surface winds at 11:00
a.m. MST, July 29, 1975.

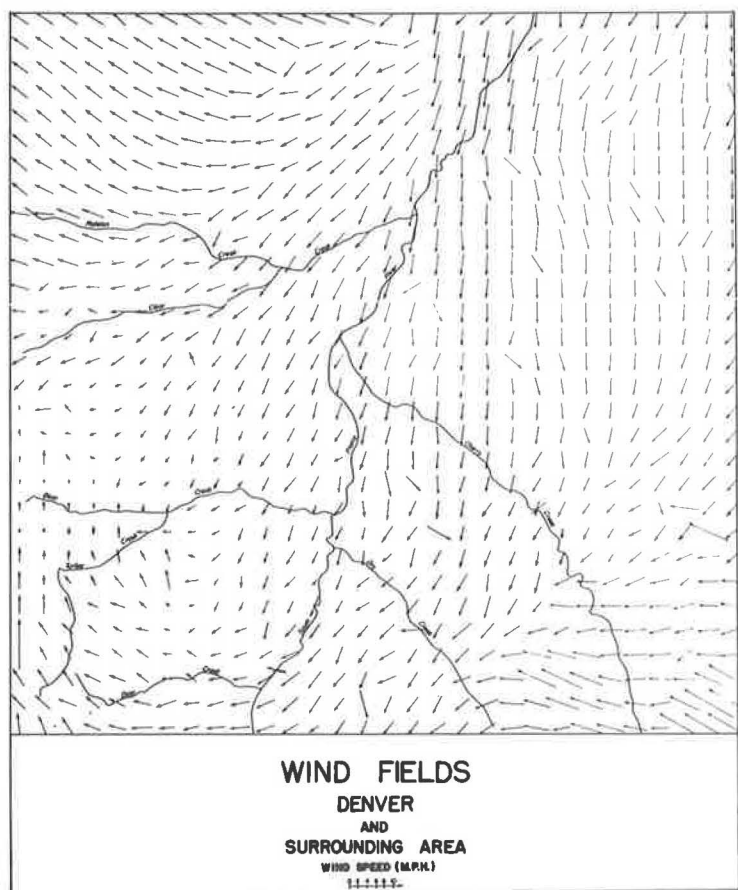


Figure 12. Systems Applications, Inc., model-generated surface winds at 5:00 p.m. MST, July 29, 1975.

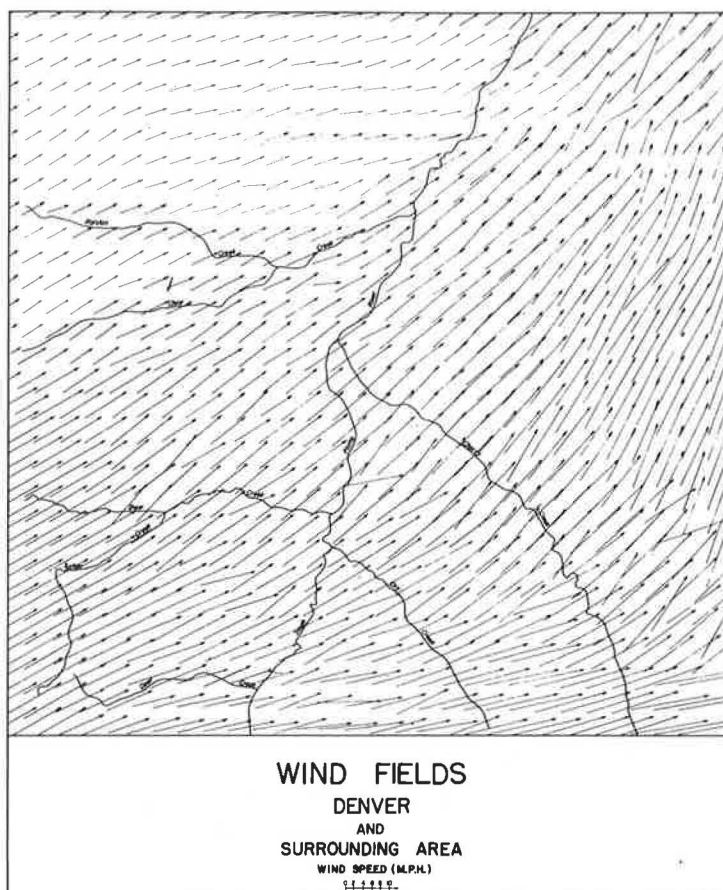


Figure 13. Typical spatial distribution of pollutants as predicted for Denver: second highest 1-h CO concentration.

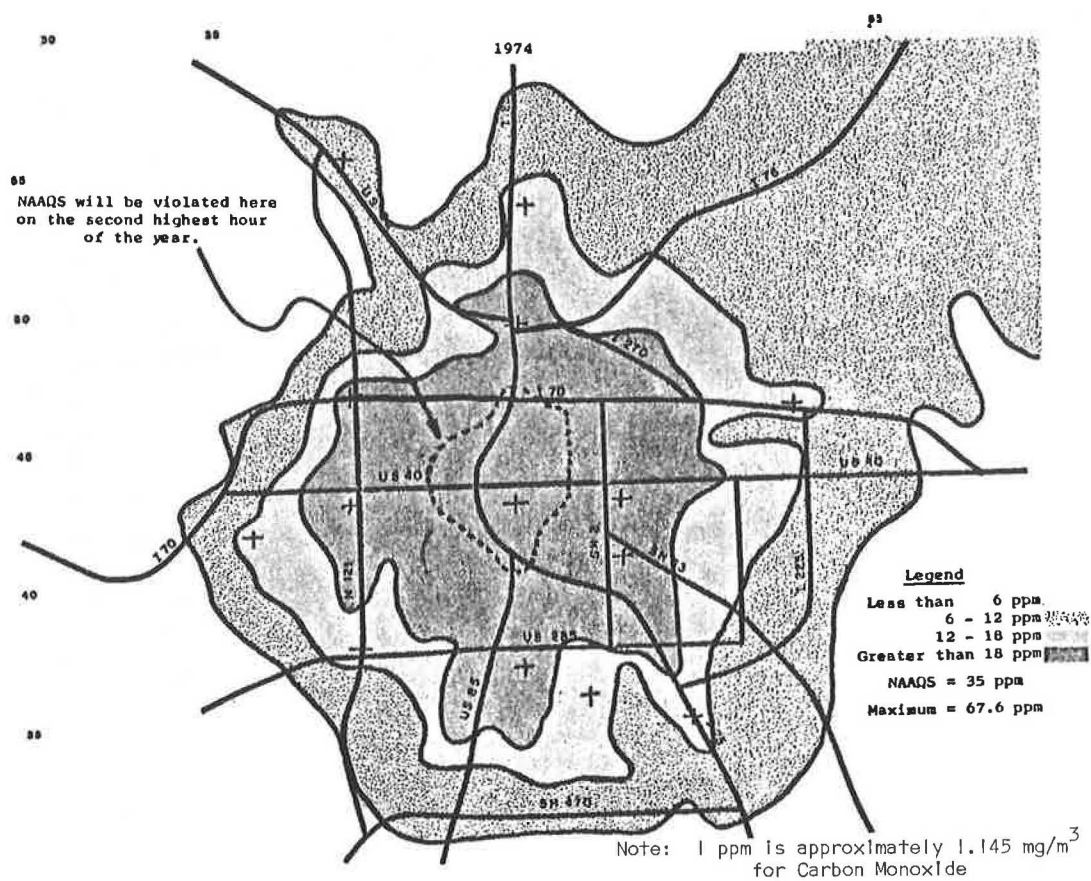
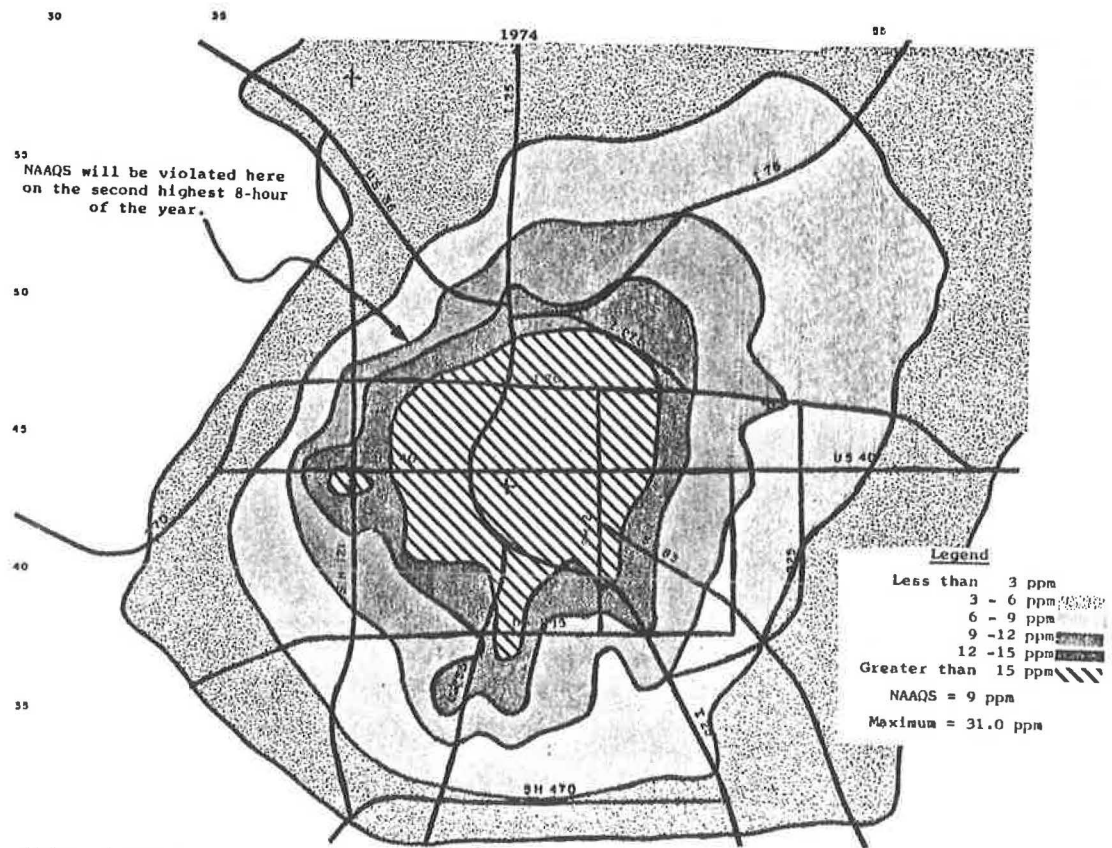
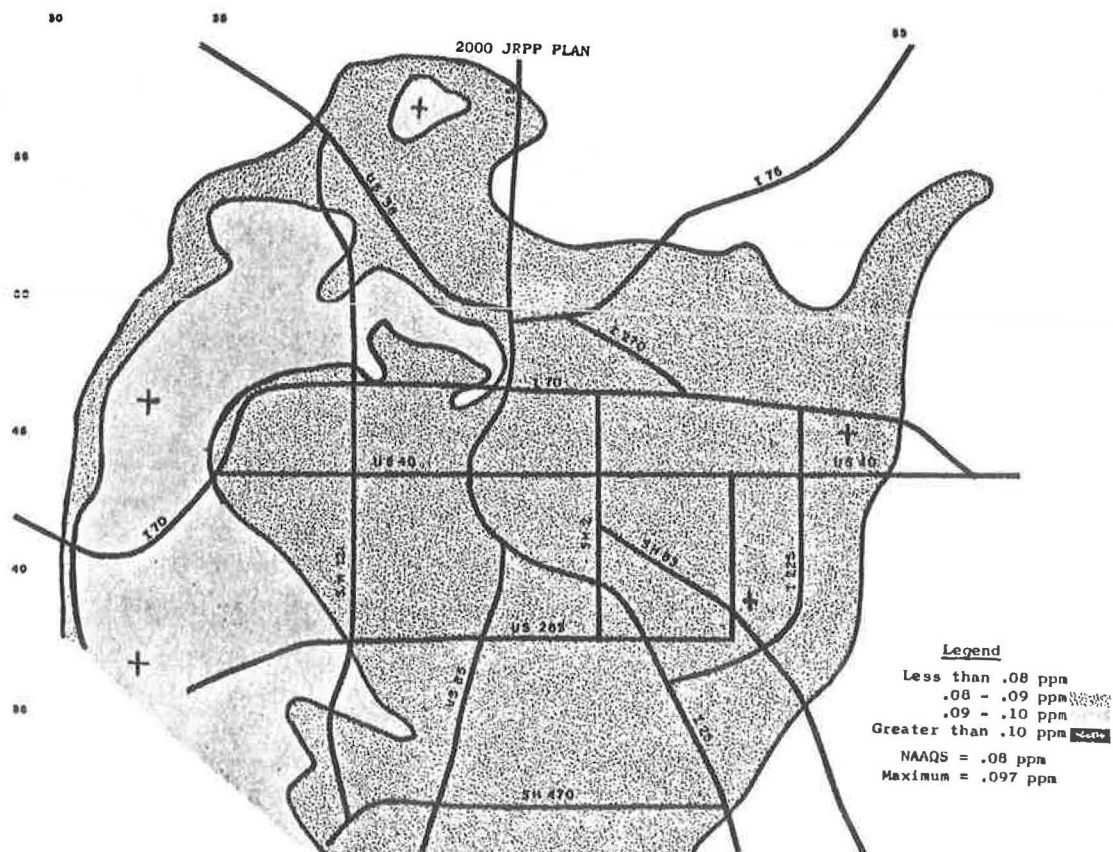


Figure 14. Typical spatial distribution of pollutants as predicted for Denver: second highest 8-h CO concentration.



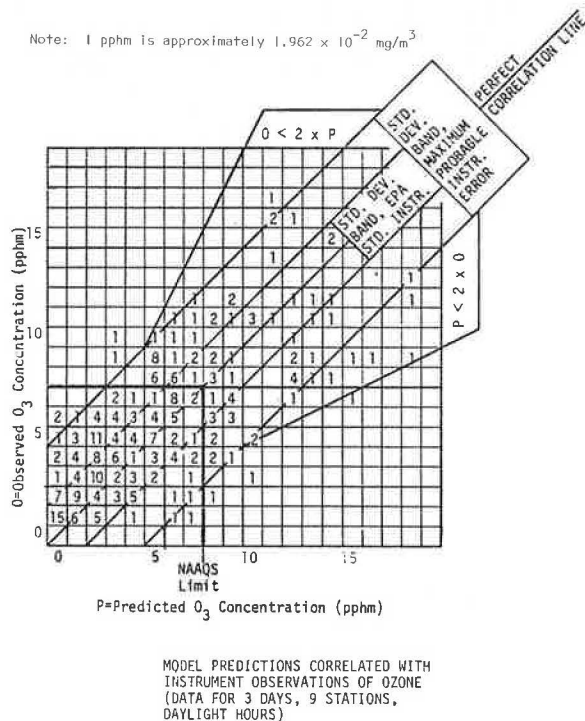
Note: 1 ppm is approximately 1.145 mg/m^3 for Carbon Monoxide

Figure 15. Typical spatial distribution of pollutants as predicted for Denver: maximum 1-h O_3 concentration.



Note: 1 ppm is approximately 1.962 mg/m^3 for Ozone

Figure 16. Denver model predicted O₃ correlated with observations.



Planned Revisions

During the past 2 years, considerable experience has been gained in the application of photochemical models to the Denver area. During 1975, the original version of the System Applications, Inc., model was adopted. Subsequently, during 1976 to 1977, System Applications, Inc., conducted a study sponsored by EPA (5) to examine the influence on air quality of urban growth associated with the availability of new wastewater treatment facilities. An updated version of the model was applied for this effort. System Applications, Inc., is currently engaged in further model-evaluation studies under a contract from the FHWA. Similarly, engineers and environmentalists from the Colorado departments of health and highways have gained expertise in the operation and application of photochemical models. This expertise has led to minor model adjustments that better simulate conditions in Denver, expansion in the monitoring network in the Denver area, and continuation of the search for a day to calibrate the model under conditions of worst case air quality.

The Colorado departments of health and highways plan to adapt the model as used in the EPA study for use in evaluating transportation alternatives. This later version of the model (including a 39-step chemistry) will be executed on the CDC 7600 computer system at the Lawrence Berkeley Laboratory in California. (The conversion from the 15-step chemistry exceeds the capacity of the CDC 6400 computing system currently being used at the University of Colorado.)

The use of the new, second-generation model for the EPA contract revealed some flaws in the model that was originally used in Denver. The revised model, commonly referred to as the Denver model, considers a 12-species chemistry, including aldehydes. Now that the comparison has been made, the new chemistry must be used if we are to attempt to model the realities of urban atmospheres.

The use of the revised model has been demonstrated to be more reliable when predicting photochemical oxidants (O₃). Although background concentrations of O₃ are not well determined (low background concentrations are difficult to measure accurately), the higher concentrations are more predictably distributed. The Denver model appears to be capable of reproducing a representative distribution of the higher, and thus more important, O₃ concentrations. The correlation between observed and predicted O₃ concentrations is shown in Figure 16. The numerical correlogram in this figure shows the number of occasions for which any particular combination of observed and predicted concentrations was obtained. Observations and predictions would be perfectly correlated if all points were on the diagonal through the origin. The points, in fact, lie generally along the diagonal but spread substantially about that line. This spread of points from the diagonal indicates that, except for a small underprediction at the lowest concentrations, the mean fractional deviations are modest and, apparently, random. These data do not confirm any finding of systematic error in the simulations.

The comparison between observed and predicted values of O₃ improves when individual sites are averaged. Data similar to that displayed in Figures 8 and 9 were averaged over all days correlated with the Denver model. When the data were averaged over time of day, all days, and stations, the average prediction was found to be just 0.8 mg/m³ (0.4 ppm) less than the average observations. Of course, this averaging process hides individual differences. However, no basic shortcomings in the model are identified by this measure.

Cost

The cost to run this program varies, depending on the computing facilities and the area being studied. The air quality simulation performed in the Denver metropolitan area was run on a Control Data Corporation 6400 computing facility that had input from a 30 x 30 grid of approximately 15 000 traffic links. The data preparation programs consisting of allocation of emissions into grid cells, meteorological distribution, and others are executed and used as input to the air quality simulation program. These preparation programs constitute 10 percent of the total cost for photochemical oxidant simulations and 25 percent of the total cost for CO-only simulations. All preparation programs need not be run for each simulation, however.

The version of the Systems Applications, Inc., program run on the CDC 6400 requires approximately 41 000 words in central memory and takes approximately 25 central processor unit (CPU) min/h of photochemical simulation. If only CO concentrations are desired, the photochemistry can be bypassed and concentrations can be computed using approximately 1.5 CPU min/h of simulation. Using the Colorado Department of Highway's CDC system, this translates into \$300/h for oxidant runs and \$25/h for CO runs during prime computing time.

CONCLUSION

The Systems Applications, Inc., photochemical model is easily adapted to urban areas. This is especially true when transportation assignments are available for the roadway network, a stationary source emission inventory exists, and a reasonable meteorological data base is available. The model is a very good predictor of the 1-h and 8-h average CO concentrations by grid cells in the Denver area. The model, as used in the past, adequately predicts O₃ concentration in order to address the NAAQS. The revised Denver model improves this capability to

where it approaches the accuracy of on-line monitoring equipment.

Model outputs are comprehensive and adequately address a system analysis throughout an airshed region. The model can be useful for determining impacts from alternative major transportation facilities, transportation system concept variations, and proposed air pollution control strategies. Revisions in model capabilities and accuracy are being made continuously; however, care should be exercised to avoid a model that is beyond the state of the art for pollution monitoring and requirements for data base inputs.

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Photochemical Oxidants in Phoenix

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The standard for photochemical oxidants is often exceeded during the summer in the Salt River Valley in the vicinity of Phoenix. Assessment of the photochemical oxidant problem in Phoenix is complicated by relatively low concentrations of nitrogen oxides in the morning, winds that switch direction in the middle of the day, and large changes in mixing height. In this paper, current measurements, modeling efforts, and control strategies are discussed as they apply to Phoenix. Although linear rollback or semiempirical correlations based on smog-chamber or actual measurements are now used to evaluate transportation strategies, better results could be obtained from mathematical air pollution simulation models. The linear rollback analysis currently used by local transportation planners shows that continued inspection and maintenance programs for automobiles and some vapor recovery programs will be required to reduce the maximum photochemical oxidant concentrations in Phoenix to levels below standard. The purpose of this paper is to review the current status of the photochemical oxidant problem in Phoenix and to make projections for the future.

Although the 1-h photochemical oxidant standard is often violated during the summer months in Phoenix, the frequency of violations varies considerably from year to year. Some form of control of nonmethane hydrocarbon (NMHC) and nitrogen oxide (NO) emissions is necessary to reduce the photochemical oxidant concentrations in the future. A limited amount of measurement data indicates that approximately a 50 percent reduction in NMHCs will be necessary by 1982.

In 1974, the Phoenix standard metropolitan statistical area was designated an air quality maintenance area for carbon monoxide (CO) and photochemical oxidants. Since then, considerable effort has been expended by the state departments of transportation and health services and the U.S. Environmental Protection Agency (EPA) to prepare an implementation plan for Phoenix. Yearly revisions will require continuous evaluation of the progress toward attainment of the standard.

PHOTOCHEMICAL OXIDANT MEASUREMENTS

A long-term record is available at only one location in Phoenix; however, in 1974 the method of analysis was

changed from continuous colorimetric to continuous ultraviolet absorption. Thus, comparisons between pre- and post-1974 data may not be meaningful. At the central Phoenix location maintained by Maricopa County, the number of violations of the 1-h oxidant standard of $160 \mu\text{g}/\text{m}^3$ and the number of days on which the violations occurred are shown in Figure 1 for 1967 through August 1977. Clearly, more information is needed to evaluate the trends. The maximum measured hourly average concentration showed a drop from approximately $370 \mu\text{g}/\text{m}^3$ to $250 \mu\text{g}/\text{m}^3$ from 1973 through 1976 at the same central Phoenix location. However, in 1976 Aerovironment, Inc., performed a study at two locations, one about 19 km southwest of this site and the other 19 km east; a maximum con-

Figure 1. Number of times and number of days the oxidant standard was exceeded for the years 1967 through August 1977 at the Phoenix central station.

