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The Sensitivity of Complex Photochemical Model Estimates To Detail In Input Information

Appendix B - Specification And Assessment Of Airshed Model Input Requirements

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Office of Air Quality Planning and Standards
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Appendix B

SPECIFICATION AND ASSESSMENT OF AIRSHED MODEL INPUT REQUIREMENTS

Systems Applications, Inc. (SAI) has been engaged in a research study sponsored by the Environmental Protection Agency (EPA) to evaluate the use of non-data-intensive methods for assessing the effectiveness of state implementation plans (SIPs) for controlling photochemical oxidants. The need for this work stems largely from the revisions to the SIPs that are required by 1982. Because the immediacy of such a deadline places serious practical constraints, both upon those formulating the revisions and those asessing them, it appears worthwhile to explore the use of complex air quality simulation models (AQSMs) as a means of assessing the adequacy and accuracy of simpler oxidant prediction methods.

This appendix reviews the input requirements of the SAI Urban Airshed Model--a three-dimensional, time-dependent photochemical dispersion model. Levels of detail characteristic of model input data are discussed and estimates of data acquisition costs are made. (These estimates are subject to change caused by regional differences in construction and maintenance costs, labor costs, inflation, etc.) Finally, the results of recent photochemical grid model sensitivity studies are presented to provide a perspective on the sensitivity results discussed in the main body of this report.

1. A REVIEW OF AIRSHED MODEL INPUTS

The objective of this review is to define comprehensively the many data inputs required by a complex photochemical grid model and to interpret the extensive model output information. Although several photochemical dispersion models now exist, the model recently refined by SAI under EPA Contract 68-02-2429 (the so-called EPA-5 model) was selected primarily because it has the most extensive input requirements of any operational photochemical model developed to date.

Airshed model inputs can be broadly categorized as either data related or nondata related. The list in table B-1 are non-data-related model inputs. Many of the inputs listed in table B-1 can be prepared

TABLE B-1. INPUT PARAMETERS FOR THE SAI URBAN AIRSHED MODEL*

Control Parameters	Chemistry Parameters
Region description:	For each species:
UTM coordinates of grid origin	Name
Cell size; horizontal and vertical	Reactive or unreactive
Grid size	Steady-state initial conditions
Number of vertical layers	Steady-state boundary conditions
Simulation controls:	Resistance to deposition
Run identification	Upper and lower bounds on numerical integration and steady-state calculations
Beginning and ending times	For each reaction:
Time step size	Rate constant
Minimum time step	Photolysis rate
Convergence criteria	Temperature dependence
Averaging interval	Activation energy
Instantaneous output interval	Reference temperature
Print options	For each coefficient:
	Name
	Value

* Ames, J., et al. (1978) discuss the airshed model inputs in considerable detail.

without recourse to air quality measurements, emission information, and so forth. Specification of certain input parameters, however, does require some knowledge of the unique conditions surrounding a given model application. For example, if the model is to be applied to a city containing several large elevated point sources, then some estimate of the diurnal distribution of plume rises must be made so that the top of the modeling region is high enough to contain point sources emissions. Clearly, in estimating the distribution of plume rises, one must have some information about the meteorology of the region and the physical emission characteristics of the sources.

Data-dependent input requirements of the SAI Airshed Model are summarized in table B-2, which indicates the spatial and temporal resolution of each input. The resolution of each input corresponds to the present configuration of the model. The indicated resolution is, in some cases, greater than that required to operate the model and to obtain acceptable simulation results. Moreover, the resolution identified in table B-2 does not necessarily represent the maximum level of input information detail that could potentially be used in a photochemical simulation. A few examples of this point are discussed next.

Atmospheric stability is characterized as the Airshed Model by three scalars: the temperature gradient below the base of the inversion (the so-called "diffusion break"), the gradient through the stable layer, and the exposure class. (The exposure classification is similar to, though not exactly the same as, the Pasquill-Gifford stability categories.) These inputs are used in the model diffusivity and plume rise algorithms. Focusing on the first two scalars, one can see that for some applications, the vertical gradients in ambient temperature vary from place to place. The Los Angeles air basin is an example. Surface temperatures near the coast are moderated by moist marine air, whereas near the eastern end of the basin hot, dry, desert-like conditions prevail. Moreover, the rate of adiabatic heating caused by air mass subsidence varies across the basin, in part because of the higher water content of the marine air. Thus, the temperature gradients in the mixed and stable layers are expected to exhibit spatial as well as temporal variability. Owing to the paucity of upper air temperature soundings, however, the temperature structure is currently treated in the model as scalar quantities, varying only in time.

Radiation intensity is another meteorological variable that is treated as a scalar. Despite the findings of photochemical model sensitivity studies, which consistently demonstrate the important role of solar radiation in oxidant formation, radiation is treated as a scalar value rather than a three-dimensional, time-varying field. For model applications in which large portions of the region experience partial obscuration

TABLE B-2. SUMMARY OF DATA-DEPENDENT INPUT REQUIREMENTS OF THE SAI URBAN AIRSHED MODEL (EPA-5 VERSION)

Description	Spatial and Temporal Resolution				Remarks
	xy	xyz	z	t	
Meteorology					
Horizontal (u-v) winds (m/sec)		x		x	The vertical component, w, is computed by the airshed model, rendering the resultant wind field mass consistent
Reference height of surface wind monitoring stations (m)	x			x	Used in the diffusivity algorithm
Diffusion break (m)	x			x	Elevation at which the stability structure of the atmosphere changes markedly (e.g., an inversion or thermal internal boundary layer)
Top of modeling region (m)	x			x	
Ground-level temperatures (°C)	x			x	Not absolutely essential to model operation
Atmospheric pressure (mb)				x	
Temperature gradient below diffusion break (°C/m)				x	Used in plume rise calculations
Temperature gradient above diffusion break (°C/m)				x	Used in plume rise calculations
Water concentration in the atmosphere (ppm)				x	Used in kinetic module
Exposure (stability class)				x	Used in diffusivity algorithm
Radiation intensity factor (per min)				x	Used in kinetic module
Air quality					
Initial conditions (pphm)		x		x	Required for NO, NO_2, O_3, HNO_2, H_2O_2, olefins, paraffins, aldehydes, aromatics, PAN, SO_2, $SO_4^=$, and CO
Boundary conditions (pphm)		x		x	Required for same species as above
Concentrations above top of modeling region (pphm)	x			x	Required for same species as above
Surface concentrations at several locations within modeling region (pphm)	x			x	Required for verification and evaluation of model performance (same species as above)
Surface characteristics					
Surface roughness (cm)	x				Used in diffusivity, surface sink, and microscale algorithms
Vegetation factor	x				Used in surface sink algorithm

TABLE B-2 (Concluded)

Description	Spatial and Temporal Resolution				Remarks
	xy	xyz	z	t	
Emissions					
Lumped ground-level emissions from traffic, area sources, airports, etc. (gm/hr)	x			x	Required for NO, NO_2, O_3, HNO_2, H_2O_2, olefins, paraffins, adehydes, aromatics, PAH, SO_2, $SO_4^=$, and CO
Elevated stationary point source emissions (gm/hr)				x	Emissions from tall stacks for the above species are required
Elevated mobile source emissions (gm/hr)		x		x	Emissions from aircraft takeoffs and landings for the above species are required (as appropriate)
Location and height of elevated point source emissions (m)		x			Required for computation of effective stack heights
Location of aircraft flight areas (m)		x		x	Requirement depends on magnitude of aircraft emissions
Heat flux from elevated point sources (cal)				x	Used in plume rise algorithm
Roadway emission rates from autos (gm/hr)	x			x	Required for NO, NO_2: used in the treatment of subgrid-scale (mino-scale) phenomena
Roadway microscale parameter (m/sec)	x			x	Parameter given by $\sum_i n_i v_i$, where i = vehicle type, n_i = number of vehicles in category i, and v_i = speed of vehicles in category i

(as a result of clouds, haze, and so forth), spatial variation in solar radiation may be important. Although current routine field measurements do not allow the preparation of three-dimensional radiation fields, the model's formulation does attempt to account, at least in principle, for the vertical attenuation of solar radiation caused by aerosol scattering.

The prescription of initial and boundary conditions is another area in which the model could accept more sophisticated input information if it were available. Currently, total hydrocarbon concentration measurements (or alternatively, nonmethane hydrocarbons) are apportioned among five reactivity classes--olefins, paraffins, carbonyls, aromatics, and ethylene. The relative fraction of each class is assumed to be spatially and temporally invariant. For a homogeneous hydrocarbon source distribution, this approach is reasonable, as long as the estimate of each species fraction is accurate. In the absence of any hydrocarbon speciation measurements, and particularly for a varied source distribution (e.g., refineries, automobiles, dry cleaners) such an apportionment scheme can potentially degrade model performance. Specifically, it might increase or decrease the oxidant maxima and alter the phasing of the formation of secondary pollutants.

A final example of refined inputs that could be accepted by the model if they were available, concerns the treatment of ground-level emissions. Currently, the emission data file (EDF) lumps (for each ground-level grid cell) all surface emissions into one emission rate, regardless of whether the emissions are from airports, autos, refineries, rendering plants, and so forth. If the goal of the modeling effort is to assess the level of model accuracy and precision, this lumping procedure is adequate only as long as the aggregate emission value is correct. But, if the modeling objective is to assess the effectiveness of a specific control strategy (say, a 60 percent reduction in refinery hydrocarbon emissions), then it becomes necessary to modify the EDF to reflect such a scenario. If gridded emission inventories are available that delineate each source type, the model can readily accept the increased level of detail.

2. ESTABLISHMENT OF CHARACTERISTIC LEVELS OF INPUT DATA DETAIL TO BE EXPECTED FOR A RANGE OF MODEL APPLICATIONS

Efforts performed under this task were twofold. First, a brief review of the status of data acquisition activities was carried out in the following 14 cities:

- Albuquerque, New Mexico
- Chicago, Illinois

- Denver, Colorado
- Houston, Texas
- Las Vegas, Nevada
- Los Angeles, California
- New York, New York
- Philadelphia, Pennsylvania
- Phoenix, Arizona
- Portland, Oregon
- Sacramento, California
- San Francisco, California
- St. Louis, Missouri
- Washington, D.C.

The purpose of this review was to develop a general understanding of the spectrum of urban-scale air monitoring activities throughout the United States. The cities that were selected shared several attributes. They were:

- Moderate to large in size.
- Representative of major geographical areas in the contiguous 48 states.
- Reflective of a variety of emission source activities, including emphasis on transportation (Los Angeles), petrochemical (Houston), light density residential (Sacramento), heavy density residential (New York), heavy industry (St. Louis), and other activities.
- Subject to exceedances of the one-hour federal oxidant standard, in some cases by a factor of 2 or 3.

Furthermore, some of the cities that were selected have been the subject of previous or ongoing photochemical modeling studies, thereby making it possible to develop a more complete picture of the available data base.

Investigation of the data bases of these cities was made through telephone discussions and correspondence with many people, principally officials from the EPA offices, state agencies, local air pollution control agencies, and other individuals who had modeling experience in certain of the cities. The results of this brief review are presented in three parts in table B-3: meteorological, air quality, and emission inventory data. Blanks in the table indicate that the information was either unavailable or not readily accessible.*

As expected, a wide range of number and type of measurements was encountered. All cities have at least a few surface wind stations, but the range in the amount of available upper level wind and atmospheric stability data is very broad. Contrast, for example, St. Louis with Phoenix or Houston. The amount of air quality monitors also varies and, to a degree, reflects the predominant air quality concern in each city. Note that oxidant monitoring in St. Louis and Los Angeles is extensive, whereas in Las Vegas concern seems to focus more on carbon monoxide. Insofar as this brief review could determine, none of the cities investigated routinely carry out hydrocarbon speciation experiments or airborne air quality measurements, though these measurements were sometimes reported during occasional special field studies.

In table B-3, the area of greatest uncertainty is the chartacterization of the emission inventories. Often, the individuals responsible for supervising the collection of air quality and meteorological data were not involved in preparing emission inventories. Because the scope of this review ruled out a detailed characterization for each city, it was occasionally necessary to rely on the general understanding of certain people of the emissions data base rather than speaking directly with the person or persons who prepared each one. From table B-3(c), it is clear that great variation exists from city to city in terms of the thoroughness and complexity of the emission inventories. As an example, the St. Louis mobile source inventory accounts for spatial variations in the diurnal distribution of the percentage of cold automotive starts, whereas traffic emissions in New York are determined borough by borough, based on the vehicle miles traveled (VMT).

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* One of the prominent difficulties encountered in the review was uncertainty on the part of certain officials as to the current status of the monitoring networks. Often, systems were being dismantled, brought on line, or used only during special studies. In addition, some agencies (or local air pollution control districts) were, at times, unaware of the scope of monitoring activities carried out by other groups, such as the National Weather Service, airports, the military, and educational institutions.

TABLE B-3. SUMMARY OF ROUTINE AIR QUALITY MONITORING ACTIVITIES IN 14 MAJOR CITIES IN THE UNITED STATES

(a) Number of Stations Performing Routine Air Quality Sampling

City	Oxidant	NO_x	CO	SO_2	NMHC	Particulates	$SO_4^=$	Upper Air Measurements	Hydrocarbon Species
Albuquerque, NM	4	3	5	3	0	13	0	0	0
Chicago, IL	4								
Denver, CO	9	3	9	1	2	0	0	R	
Houston, TX	3	3	3	3	3	3			
Las Vegas, NV	3	2	24	0	4	3	0	0	0
Los Angeles, CA	39	27	23	17	11		8	R	S
New York, NY	7	7							
Philadelphia, PA	8	5	8	8	3	8			
Phoenix, AZ	5	2	8		3				
Portland, OR	3	3	15						
Sacramento, CA	8	8	8		4	1	0	0	
San Francisco, CA	26	16	16	21	16	17	17	0	
St. Louis, MO	25	25	25	11	25	20	10	S	S
Washington, D.C.	10	10	10	10	10	10			

S = special studies.

R = rarely.

Note: A zero entry indicates that a particular measurement is not taken; a blank indicates uncertainty as to whether or to what extent the measurement is taken.

TABLE B-3 (Continued)

(b) Number and Type of Daily Meteorological Measurements

City	Surface Wind Velocity	Surface Temperature	Atmospheric Stability	Upper Level Wind Velocity	Solar Insolation	Humidity
Albuquerque, NM	7	7	Rw_1	Rw_1	1	1
Chicago, IL	10	10	Rw_2	Rw_2	3	3
Denver, CO	25	2	Rw_1	Rw_1	1	1
Houston, TX	3	3	0	P_1	1	1
Las Vegas, NV	8	1	AC_2, AS_1	0	1	1
Los Angeles, CA	44	9	RD_8, AS_1	RD_8	2	8
New York, NY	10	10		P_1	3	3
Philadelphia, PA	2	2		P_1	1	1
Phoenix, AZ	8	8	0	0	1	1
Portland, OR	9	9	Rw_1	Rw_1, P_1	1	1
Sacramento, CA	12	4	AS_3	P_4	1	2
San Francisco, CA	17	17	Rw_1	Rw_1	17	17
St. Louis, MO	25	25	RD_8	P_{96}	6	20
Washington, D.C.	25	25	Rw_1	Rw_1	2	2

AC = acoustic sounder.

AS = aircraft spiral.

RD = radiosonde.

Rw = rawinsonde.

P = pibal.

Notes: Subscripts refer to the number of measurements taken each day. A zero entry indicates that a particular measurement is not taken; a blank indicates uncertainty as to whether or to what extent the measurement is taken. In some cases, the meteorological measurements presented here were drawn from special studies conducted during the summer smog season; in other cases only routinely collected data are presented.

TABLE B-3 (Concluded)

(c) Description of Methods Used for Emission Inventories

	Motor Vehicle Emission Inventory				Point and Area Sources Emission Inventory			
City	Format	Species	Grid Size	Hot/Cold Start	Format	Species	Spatial	Temporal
Albuquerque, NM	Link-node: VMT	N, H, C	N/A	Area-wide temporal resolution	NEDS	N, H, S, P, C	Area-wide	Annual average
Chicago, IL	Gridded	N, H, C	50 x 50: 2 mi		Gridded	N, H, C	2 mi	
Denver, CO	Gridded	N, H, S, P, C	30 x 30: 1 mi	Area-wide temporal distribution	Gridded	N, H, S, P	1 mi	8 or 24 hour, plus seasonal
Houston, TX	Link-node: VMT				By counties	H, S, H, P	County-wide	
Las Vegas, NV	Gridded	N, H, C	30 x 40: 1 km	Area-wide temporal distribution	Gridded	N	1 km	
Los Angeles, CA	Gridded	N, H, S, C	100 x 50: 2 mi	Area-wide temporal distribution	Gridded	N, H, S, C	2 mi	Hourly
New York, NY	VMT		Borough by borough			S, P		
Philadelphia, PA	Gridded	H, C, N	48 x 48: 2 mi		NEDS	N, H, S, P, C	Area-wide	Annual average
Phoenix, AZ	Gridded	N, H, C	1 mi		NEDS	N, H, S, D, C	Area-wide	Annual average
Portland, OR	Gridded	S, P, C	20 x 30: 2 km		By district	H, N	Depends on size of districts	
Sacramento, CA	Gridded	N, H, S, P, C	25 x 25: 2 km	Area-wide temporal resolution	Gridded	N, H, S, P, C	2 km	Annual average
San Francisco, CA	Gridded	N, H, S, P, C	120 x 60: 1 km	Area-wide temporal distribution	Gridded	N, H, S, P, C	1 km	Hourly
St. Louis, MO	Variable size grid	N, H, S, P, C	150 x 200: 1-10 km	Hot/cold distributions applied to each grid cell	Gridded	N, H, S, P, C: hydrocarbon speciation	1-10 km	Hourly
Washington, D.C.	Gridded	N, H, S, P, C	4 mi		Gridded	N, H, S, P, C	4 mi	

N = nitrogen oxides.

H = hydrocarbons.

S = sulfur oxides.

P = particulates.

C = carbon monoxide.

Delineation of characteristic levels of detail in the data available for photochemical modeling was attempted, once the foregoing assessment of present urban-scale data bases was complete. With this review as a guide, and realizing that certain measurements are clearly beyond the scope of routine monitoring practices, table B-4 was formulated, yielding three general "levels of detail" of data input to a complex model. Associated with each of nine types of input information are statements reflecting the type and amount of data one might expect for each level of detail. The "maximum practical level" corresponds to the most extensive data base that is currently available or that might be made available given present funding constraints and the state of the art in photochemical modeling. In many respects, the St. Louis and South Coast Air Basin data bases are examples of this category.

At the other end of the spectrum is the "minimum acceptable level." Although a data base so characterized might be adequate for modeling purposes, certain assumptions must necessarily be invoked in preparing model inputs. For example, Phoenix has no upper air temperature soundings. To estimate mixing depths over Phoenix, one might assume that the atmospheric structure at Tucson (where upper air soundings are available) is reflective of conditions over Phoenix. Although mixing depth estimates might be generated in this fashion, the extent to which they degrade model performance and thus confound model performance evaluation efforts is unknown. Between these two levels of detail lies a third category entitled "commonly used level." Most of the data bases presented in table B-3 fall within this category. This does not suggest, however, that these data bases are well suited to model performance evaluation and application. Some of the measurements that are either lacking or in short supply in the intermediate category are ones to which model performance is quite sensitive.

3. ESTIMATION OF DATA ACQUISITION COSTS ASSOCIATED WITH RAISING THE LEVEL OF DETAIL OF INPUT DATA

The objective of this analysis was to derive preliminary estimates, where possible, of the costs entailed in improving the quantity, quality, or both of various components of an AQSM data base over that currently being collected. If, in fact, one can identify the improvement in model performance achieved through data from an additional wind station or pyranometer, for example, then this could serve as the basis for quantifying the degree of improvement in model performance ascribable to a specific expenditure.

Relatively little in the recent literature serves as a guide in this endeavor. One might expect that the lack of guidance is in part a result

TABLE B-4. LEVELS OF DETAIL IN DATA USED AS INPUT TO GRID-BASED AIR QUALITY SIMULATION MODELS

Input	Maximum Practical Level	Commonly Used Level	Minimum Acceptable Level*
Atmospheric stability	Continuous monitoring of mixing depths with acoustic sounder at one or more locations Several (5-8) vertical temperature soundings throughout the day at various locations within the modeling region Numerous surface temperature measurements recorded hourly at various locations throughout the modeling region One or more instrumented towers providing continuous measurements of the mixed layer thermal structure	A few (3-5) temperature soundings at different times of the day at one or two locations Several surface temperature measurements recorded at various locations throughout the modeling region	Twice daily temperature soundings at an airport within or nearby the region being modeled A few (1-3) surface temperature measurements with which to estimate temporal variation Limited spatial resolution or none at all
Wind fields	Numerous ground-based monitoring stations reporting hourly average values Frequent upper air soundings at several locations throughout the modeling region Continuous upper level measurements on one or a few elevated towers Wind, inversion, temperature, and terrain data used as input to the 3-D numerical model yielding the mass conserving 3-D wind field	Interpolations from ground-based monitoring network and limited (3-5) number of upper level soundings at one or two locations Resultant wind field rendered mass consistent by divergence-free algorithm	Interpolations from limited (3-5 stations) routine surface wind data; theoretically derived vertical profile assumed
Solar radiation	Several (3-5) UV pyranometers located in the region, continuously recording UV radiation levels Vertical attenuation of radiation at a few locations several times daily determined by aircraft observations Spatial (3-D) insolation fields determined by interpolation of measurements	A single, ground-based net radiometer; insolation assumed constant over the region Vertical attenuation estimated empirically as a function of aerosol mass	No radiation measurements available; estimated theoretical values based on the solar zenith angle Attenuation not accounted for
Boundary and initial conditions	Hourly species concentrations extrapolated and interpolated throughout the region using data from the extensive ground-based monitoring network; airborne data also available; hydrocarbon mix obtained from gas chromatographic analyses at several times during the day Sulfate concentrations available on an hourly basis at several locations	Hourly concentrations extrapolated and interpolated using data from several ground-based stations; hydrocarbon mix obtained from gas chromatographic analysis at one or two stations one or a few times during the day Sulfate concentrations based on a daily average and diurnal ozone curve	Hourly concentrations extrapolated and interpolated from a minimal routine monitoring network; either hydrocarbon mix assumed or average value obtained from a compilation of available data taken in a similar area No data on concentration variations aloft Sulfate measurements inferred from values obtained in similar areas

TABLE B-4 (Concluded)

Input	Maximum Practical Level	Commonly Used Level	Minimum Acceptable Level*
Stationary source emissions	Separate gridded inventories for point and area stationary sources; characterization of organic composition, and NO/NO_2 and SO_2/SO_4 emission rates for major sources; diurnal and seasonal variations in nominal emission rates for each major source type	Lumped, gridded inventory for stationary sources; NO species fractionation; seasonal and diurnal variation in regional emissions for each pollutant	Lumped stationary source emission inventory for the region as a whole; limited information on the percentage of each source type; no temporal variation
Hydrocarbon species distribution	Mix obtained from gas chromatographic analysis of samples collected throughout the region, particularly near large sources Cold start factors applied grid by grid when calculating mobile source emissions	Mix obtained from standard emissions factors (AP-42) together with a detailed source inventory, supplemented with one or two gas chromatographic analyses	Mix assumed or obtained from available data compilation, either for the city of interest or some similar area
Mobile source emission factors	AP-42 (latest supplement) emission factors used in conjunction with local vehicle age distribution; corridor-by-corridor VMT, including peak and off-peak speed distributions, vehicle mix, and traffic data for intrazonal trips	AP-42 emission factors, assumed vehicle mix, and intrazonal VMT; estimated peak and off-peak speeds, fewer traffic counts available for verification, VMT available for fewer major arterials	Gridded VMT, emission factors estimated from 49 state mix, and average (FDC) driving profile; assumed regional speed distribution
Vehicular cold start distribution	Spatial and temporal distributions of cold starts inferred from actual traffic and demographic data	Cold starts temporally resolved using traffic distribution; no spatial resolution or spatial resolution only from estimates of driving patterns	Cold starts as a fixed percentage of all driving--traffic data are not detailed enough for spatial resolution of cold starts; cold starts estimated from demographic data
Data for model performances evaluation	Hourly averaged species concentrations for NO, NO_2, O_3, SO_2, NMHC, sulfate, CO, and particulates from an extensive ground-based monitoring network	Hourly averaged concentrations of NO, NO_2, O_3, SO_2, NMHC, CO, and particulates from several ground-based stations Daily averaged sulfate measurements available from a limited (3-5) number of stations	Hourly averaged concentrations of NO_x, O_3, THC, SO_2, and CO from a minimal routine monitoring network

* Using data at this level of detail necessitates numerous assumptions.

of broad geographical variations in labor rates, operating costs, and so forth, and the ever-increasing cost of capital equipment, parts, and supplies. An earlier study for the EPA (Miedema et al., 1973) addressed the cost of implementing air quality monitoring networks of various sizes in metropolitan areas where little if any monitoring previously existed. This study, building upon earlier work by Hickey, Rowe, and Skinner (1971), estimated monitoring costs for each state in the United States for two scenarios:

> The required number of monitors based on federal regulations

> The required number of monitors based on state regulations.

The analysis carried out by Miedema et al. considered 31 cost elements when formulating overall costs for a particular network. These cost elements are listed in table B-5; as is immediately apparent, many cost categories exhibit a wide range of variation, and most costs increase in time. Accordingly, it is difficult to estimate many costs. For example, if one wind monitoring station was purchased to augment the already dense surface network in Los Angeles, the incremental costs required to train personnel, accommodate the new data in the existing data reduction and analysis system, provide for calibration and inspection equipment, and so forth would probably be low compared with the analogous costs in Houston, Texas. Along the same line, hourly labor costs in Albuquerque, New Mexico, are less than those in San Francisco, California.

Notwithstanding the difficulties in formulating cost estimates, an attempt was made to identify typical costs of routinely acquiring additional air quality and meteorological data. The results of this study are presented in table B-6. In this analysis, fixed hardware costs were amortized over a five-year period of time, but interest costs were neglected. In some cases (surface winds, for example), the variable was measured continuously; in other cases, the measurements were routine but not hourly. Twice daily radiosonde soundings are an example. The frequency of occurrence of each parameter is consistent with the maximum level of detail, outlined in table B-4.

Various sources were consulted in developing the cost figures given in table 6, including published reports, equipment manufacturers, managers of air quality monitoring networks, and researchers working on special studies. The costs for the surface air monitoring stations employing a variety of instruments should be clearly viewed as lower bounds because these figures are estimates made five years ago (Miedema et al., 1973). In discussing the cost estimates with the authors of the Miedema et al.

TABLE B-5. COST CATEGORIES FOR AIR QUALITY MONITORING SYSTEMS

(a) Fixed Costs

Hardware	Nonhardware
Remote electronics	Specification preparation and program management
Central electronics	System engineering
Test and maintenance equipment	Software
Other digital equipment	Documentation
Initial spares	Training
Site installation, physical	Site installation, APCD labor
	Site installation, vendor labor

(b) Variable Costs

Nonpersonnel	Personnel
Recurring spares	Personnel, field technician
Utilities, site	Personnel, sensor maintenance, corrective
Utilities, communications	Personnel, electrical maintenance, correction
Transportation, local	Personnel, data analyst, routine
Transportation, other	Personnel, data analyst, special
Computer rental	Personnel, laboratory technician
Supplier	Personnel, chemist
Facilities	Personnel, engineer
	Personnel, clerical
	Personnel, administrative

Source: Hickey, Rowe, and Skinner (1971).

TABLE B-6. ESTIMATED ANNUAL COST TO AUGMENT AN EXISTING AEROMETRIC MONITORING NETWORK WITH VARIOUS INSTRUMENTS

Parameter Measured	Instrument	Estimated Annual Cost
Surface wind velocity (continuously)	Remote recording cup anemometer and vane	$ 7,500
Upper level winds, temperature, relative humidity (twice daily)	Rawinsonde	71,000
Upper level winds (twice daily)	Pibal	7,000
Mixing depth (continuously)	Monostatic acoustic sounder	13,500
Mixing depth (twice daily soundings)	Light aircraft with digital recording temperature sensor	40,600
Upper level winds and temperature structure (continuous)	Instrumented tower	46,000
Solar radiation (continuous)	Pyranometer	3,800
SO_2, particulates, wind speed, wind direction	Surface air monitoring station	44,000
SO_2, particulates, wind speed and direction, CO, O_3, and NO_2	Surface air monitoring station	66,700
SO_2, particulates, wind speed and direction, CO, O_3, NO_2, total hydrocarbons, temperature, relative humidity (continuously)	Surface air monitoring station	100,000

TABLE B-6 (Concluded)

Parameter Measured	Instrument	Estimated Annual Cost
Vertical SO_2 pollutant burden (four sampling days each week during three-month smog season)	Correlation spectrometer	$ 81,000
Hydrocarbon speciation (twice daily, three times a week during three-month smog season)	Gas chromatograph	22,700
SO_2, NO_x, O_3, particulates, relative humidity, b_{scat}, turbulence, (4-5 hours daily during special field program)	Airborne air quality monitors	5,000*

* Estimated cost per day.

study, we found that no attempt has been made to revise the estimates to a more current time frame.

In some instances, it is possible to estimate the cost of additional monitors by examining current costs of data acquisition, analysis, management, and so on. The California Air Resources Board (CARB), for example, has found over the years, in comparing the overall cost of its monitoring network with the total amount of data collected, that a typical per-unit cost of data acquisition is about $1 per number. Thus, the cost of one additional hourly surface temperature measurement in an existing network might be on the order of $8,000 to $10,000 per year.

4. ANALYSIS OF AIR QUALITY MODEL SENSITIVITY TO VARIATIONS IN INPUTS

At the outset of the study (December 1977), a review of previous air quality simulation model sensitivity studies was performed. In the following subsection, the results of this review are presented. Because the photochemical grid models studied (1) represent different model structures (though they are based on the same general concept), (2) represent different levels of model refinement, and (3) were applied to different urban areas (e.g., Denver, San Francisco, Los Angeles), the sensitivity results are not directly comparable in a quantitative sense. Rather, they are indicative of trends in model performance likely to be observed when certain inputs are varied.

Within the last five years, a limited number of sensitivity studies have been performed with grid-based photochemical models. From a review of the literature, we found that only two models--the Lawrence Livermore National Laboratory LIRAQ model and the SAI Airshed Model--have undergone extensive sensitivity analyses and have had the results of these studies published in the open literature.

Table B-7 briefly summarizes recent grid model sensitivity studies. Although it is likely that other sensitivity runs have been made,* the ones identified in table B-7 are the only major sensitivity results that have been identified by this review. It is apparent from the table that several studies have investigated the impact on model predictions caused by variations in several model variables. The eight studies are aggregated according to four categories--air quality, meteorology, chemistry, and emissions--which are discussed next.

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* Indeed, in carrying out a photochemical model simulation, iterative adjustments made to initial conditions, boundary conditions, etc., constitute a form of sensitivity analysis, but these results are seldom reported formally.

TABLE B-7. SUMMARY OF SENSITIVITY STUDY RESULTS OBTAINED WITH GRID-BASED PHOTOCHEMICAL AIRSHED MODELS

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
MacCracken, M. C., and G. D. Sauter (1975)	LIRAQ photochemical model Two-dimensional time-dependent grid model Lumped kinetic mechanism similar to Hecht-Seinfeld-Dodge mechanism Mass conserving wind field	Relative humidity was reduced from 40% by 20%	Peak ozone increased by 3% and peak NO_2 decreased by 4%	LIRAQ sensitivity runs focused on the kinetic module; accordingly, sensitivity results are more reflective of smog chamber simulations than they are of airshed simulations
		Nominal temperature was increased from 285°K to 304°K	Peak ozone decreased by 2% and peak NO_2 increased by 5%	
		Light intensity was reduced by 50%	Peak ozone decreased by 70% and NO_2 peak magnitude remained unchanged but was delayed 4 hours	
		Light intensity was increased by a factor of 2	Peak ozone increased by 100% and NO_2 peak magnitude slightly increased and preceded base case peak by 1-3/4 hours	
		Initial hydrocarbons are increased by a factor of 2	NO_2 peak increased by 6% and was delayed approximately 1 hour; ozone peak was not reported, but the increase in ozone concentrations was delayed by up to 3 hours	
		Initial NO_2 concentrations were increased by a factor of 2	NO_2 peak increased by 10% and was delayed slightly; O_3 remained unchanged	
Demerjian, K. L. (1976) "EPA 3" VERSION	SAI photochemical model:	Boundary conditions were reduced by 50%	"Minor" differences occurred in ozone prediction in the eastern and northern portions of the L.A. basin; "significant" differences were observed in the western and central portions of the basin	
		Initial and boundary conditions were reduced by 50%	Predicted ozone in the northern and eastern edges of basin were reduced 20 to 30%	
Liu, M. K., et al. (1976)	SAI photochemical model: "EPA 3" version 25 x 25 x 6 grid 15-step Hecht-Seinfeld-Dodge kinetics Price numerical method Empirical diffusion algorithm Two-dimensional wind field	Wind directions were randomly perturbed by 0 or ±22.5%	A 6.9% average deviation for manually prepared and 4.9% for automatically prepared wind fields (based on CO predictions)	In the automatic wind field studies, perturbations were made to the monitoring station measurements and then automatic procedures were employed to derive gridded wind fields. In the manual wind field cases, perturbations were made to the gridded wind fields after they had been prepared manually
		Wind speeds were randomly perturbed by 0 or ±1 mph	A 4.9% average deviation for manually prepared and 2.6% for automatically prepared wind fields (based on CO predictions)	
		Wind station measurements were:	Maximum absolute deviation from the base case results for CO were	The response of the model to variations in wind speed varies with each chemical species and is time dependent

TABLE B-7 (Continued)

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
	Two-dimensional initial conditions	Increased 50%	19.6%	
		Increased 25%	11.8%	
		Decreased 20.2%		
		Decreased 50%	51.7%	
		Horizontal diffusion was decreased to 0 and increased to 500 m^2/sec	for K_H = 0, the maximum absolute deviation for CO ranged between 0.52 and 0.02% from 0600 to 1600 hours For K_H = 500 m^2/sec, the maximum absolute deviation for CO ranged between 4.4 and 12.9% from 0600 to 1600 hours	
		Vertical diffusivity was decreased to 0.5 m^2/sec and increased to 50 m^2/sec	The effect of varying vertical diffusivity by an order of magnitude was about the same as that of varying the wind speed by 25 to 50%	The base case value was 5 m^2/sec
		Mixing depths were increased and decreased by 25%	Maximum absolute percentage deviations for the increase and decrease, respectively, were: For CO, 8% and 12% For NO, 11% and 18.5% For NO_2, 8.5% and 15.5% For O_3, 11.5% and 23%	The buildup of the mixing depth variation effect is time-dependent Decreasing the mixing depth has a greater effect on the ground-level concentrations than increasing it; this result is more pronounced for reactive pollutants The effect of changing the mixing depth is not uniform over the modeling region; it varies from place to place The effect on ground-level concentrations of changing the mixing depth is roughly the same as that of changing the wind speed, as would be expected from a dimensional analysis
		Radiation intensity was increased and decreased by 30%	Maximum absolute percentage deviations for the increase and decrease, respectively, were:	The effects of varying the radiation intensity are time-dependent

TABLE B-7 (Continued)

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
			For NO, 17% and 40% For NO_2, 74% and 55% For O_3, 9% and 11%	The effect of changing light intensity is as significant as that of changing wind speed
		Emissions rate (ground based) was increased and decreased by 15%	The effects of increasing and decreasing emissions rates are almost identical; peak basin-wide average percentage changes in CO and NO_2 were about the same (6-8%)	The study results are summarized by the following ranking of the relative importance of the input parameters (A = most important and D = least important): Parameter or Variable — CO / NO / O_3 / NO_2 Wind speed — A / A / A / A Horizontal diffusivity — D / D / D / D Vertical diffusivity — C / C / C / C Mixing depth — B / B / B / B Radiation intensity — D / A / A / B Emissions rate — B / A / B / B
Reynolds, S. D., et al. (1976)	SAI photochemical model: "EPA 3" version [see Liu et al. (1976)]	Uniform wind velocities with height were compared with vertical variation in horizontal winds given by a power law formulation	The maximum average percentage deviations were: 28.5% for NO, 15% for NO_2, 24% for CO, and 14% for O_3 The maximum average deviations in pphm were: -0.35 for NO, -1.1 for NO_2, -4 for CO, and -2 for O_3 The maximum deviations in pphm were: 7.5 for NO, 15 for NO_2, 30 for CO, and 26 for O_3	The effects of including wind shear were similar to those of increasing surface wind velocities by roughly 25% because velocities within the mixed layer are increased between 20 and 70% of the surface values as a result of shear
Anderson, G. E., et al. (1977)	SAI photochemical model: "Denver" version	Wind speeds were reduced by 33%	Maximum predicted ozone increased by 4%; maximum area for which $[O_3]$ > 0.08 ppm increased by 12%	

TABLE B-7 (Continued)

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
	31-step carbon bond chemistry	Mixing depths were reduced by 33%	Maximum predicted ozone increased by 16%; maximum area for which $[O_3] \geq 0.08$ ppm increased by 7%	
	3-D wind field	Wind speeds and mixing depths were both reduced by 33%	Maximum predicted ozone increased by 33%; maximum area for which $[O_3] \geq 0.08$ ppm increased by 30%	A synergism exists between wind speed and mixing depth
	Lower microscale layer	Emissions in suburban areas surrounding Denver were reduced 25% with weighted emissions increases in other areas to make overall regional emissions equivalent to those in the base case	No difference occurred in the time, location, or magnitude of maximum ozone concentration; differences among predicted ozone concentrations in all runs were not more than 0.010 ppm in one or two grid cells at most	In each scenario, no more than 7% of the region-wide emissions were redistributed; changes of this size in the spatial distribution of emissions has little effect on secondary pollutants such as ozone
	Lamb and Liu diffusivity algorithms			
	30 x 30 x 7 grid			
	SHASTA numerical method			
	Surface removal			
	Three-dimensional initial conditions	Emissions in the Denver metropolitan area were reduced 17.5% with a proportional increase in suburban areas to make regional emissions levels equivalent to those in the base case	No difference occurred in the time, location, or magnitude of maximum ozone concentration; differences among predicted ozone concentrations in all runs were not more than 0.010 ppm in one or two grid cells at most	
Killus, J. P. (1977) (private communication)	SAI photochemical model: "Denver" version [see Anderson et al. (1977) for model attributes]	Grid spatial resolution was relaxed from 1 x 1 mile to 2 x 2 miles	The coarser grid resolution led to no noticeable change in the time to peak NO, NO_2, and O_3 concentrations; the magnitude of peak concentrations was reduced for NO (69%), NO_2 (21%), and O_3 (13%)	By the time ozone forms, its precursors have been distributed over a much greater area than their source regions; accordingly, the influence of increased grid size on ozone predictions should be less than that for primary pollutants such as NO
Anderson, G. E. (1977) (private communication)	SAI photochemical model: "Denver" version [see Anderson et al. (1977) for model attributes]	NO emissions from a point source were increased by 20% (note that the source contributes roughly 1% of the Denver regional NO_x burden)	The maximum impact of increased source emissions anywhere in the modeling region was an increase in hourly averaged NO and NO_2 concentrations (12 and 5 ppb, respectively) and a decrease in O_3 (-4 ppb)	The effect was decidedly local and did not influence peak oxidant concentrations
Attaway, L. O., et al. (1975)	SAI photochemical model: "EPA 3" version [see Liu et al. (1976)]	SO_2 emissions from a refinery in Los Angeles were increased from 0.0 tons per day to 1.4 tons per day	The estimated maximum increment in three-hour-average SO_2 (0900-1200) concentrations was 70 ppb immediately downwind of the facility; concentration differences dropped below 10 ppb at a distance of 24 miles downwind of the source	The 70 ppb value is an upper bound because the mesoscale model overestimated ground-level concentrations in the vicinity of buoyant point sources
DeMandel et al. (1979)	LIRAQ photochemical model: Two-dimensional time-dependent grid model	Emissions resolution was reduced from 5 km x 5 km to 10 km x 10 km	Region-wide maximum ozone concentrations were reduced by 10 percent from a baseline peak of 0.20 ppm	The time of occurrence of the ozone peak remained unchanged

TABLE B-7 (Concluded)

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
	Compact kinetic mechanism similar to Hecht-Seinfeld-Dodge mechanism Mass-conserving wind field	Emissions were distributed according to the demographic distribution	Region-wide maximum ozone concentrations were reduced by 25 percent; the predicted peak ozone level occurred three hours after the base case maximum	The delay in the ozone peak was attributed to a redistribution of point source NO_x emissions from industrial areas to residential areas
Souten, D. R., et al. (1980)	SAI photochemical model: "EPA 5" version [see Reynolds et al. (1979)]	Reactive hydrocarbon emissions from biogenic sources (57 percent of the RHC inventory) were eliminated from the inventory	Area-wide ozone levels on the second of a multiple-day simulation were reduced by no more than 2 ppb	For the meteorology studied, biogenic hydrocarbon emissions had no major bearing on peak calculated ozone levels
Killus, J. P., et al. (1980)	SAI photochemical model: "EPA-5" version [see Reynolds et al. (1979)]			
	SAI photochemical model: "EPA-5" [see Ames et al. (1978)] Multiple-day simulation for Los Angeles, CA	Three-dimensional initial condition field from monitoring data versus "clean air"	Essentially zero effect on second day of simulation; some effect on first day, especially in western portion of modeling region in the morning	Effects on the second day of two-day simulation are driven by emissions
			No ozone predictions above 0.2 ppm on first day; no ozone above background on second day	Effects on the second day of two-day simulation are driven by emissions
		Background hydrocarbon 0.06 ppmC versus 0.18 ppmC	No effect on ozone peaks; minor effects at some stations	Background HC has limited effects below certain point
Reynolds, S. D., et al. (1979)	SAI photochemical model: "EPA-5" version [see Reynolds et al. (1979)]	Wind fields for the airshed model were prepared using the following procedures: 1. An interpolation algorithm 2. A two-dimensional wind model 3. A three-dimensional wind model	O_3 (pphm): Procedure 1: A* -0.7, P† 6.8; Procedure 2: A 1.4, P 8.6; Procedure 3: A 0.3, P 7.6 NO_2 (pphm): Procedure 1: A -2.0, P 3.5; Procedure 2: A -1.5, P 4.0; Procedure 3: A -2.2, P 3.7	Examination of the ozone results reveals the following: Use of interpolated wind fields leads to the greatest bias toward underestimation at the highest concentration levels Compared with the interpolated and three-dimensional wind field simulations, the two-dimensional wind field simulation exhibits a greater tendency toward overestimation for most of the observed concentration range The three-dimensional wind field simulation exhibits less bias (positive or negative) overall than do the other two simulations
		Grid resolution was relaxed from 2 x 2 miles to 4 x 4 miles	Generally, a reduction in the maximum ozone concentration occurs at the monitoring stations together with a "broadening" of the diurnal ozone profile	

* Accuracy.
† Precision.

a. Studies Focusing on Air Quality Inputs

Sensitivity analyses in which air quality inputs have been varied were reported by MacCracken and Sauter (1975) and Demerjian (1976). Collectively, these studies examined perturbations in model predictions from base case simulations caused by the following changes:

> Initial hydrocarbon concentrations increased by a factor of 2.

> Initial NO_2 concentrations increased by a factor of 2.

> Boundary conditions reduced by 50 percent.

> Initial and boundary conditions reduced by 50 percent.

The measures of model performance that were used in these studies included the percentage change in the magnitude of the peak O_3 and NO_2 concentrations and the time delay in reaching peak concentrations. In each case, the overall impacts on the spatial maximum O_3 and NO_2 concentrations (in percentage variation from the base case) were far less than the changes made in initial or boundary conditions.

These early studies represent an initial step in analyzing the impact of variations in air quality inputs (i.e., initial and boundary conditions) on grid model predictions. Although they provide insight into the expected order of magnitude of changes in model predictions (at least over the range for which the inputs were varied), other issues need to be investigated:

> What is the impact on predictions caused by variations in the assumed initial and boundary condition hydrocarbon species compositions?

> What is the impact on predictions caused by variations in boundary conditions over a much wider range of concentrations than have previously been explored? In some simulations, uncertainties in boundary conditions upwind of the urban area, and pollutant concentrations in layers aloft, have been much greater than the range of values explored in sensitivity studies to date.

> What is the impact on predictions caused by various procedures* for creating initial and boundary condition fields?

> What is the impact on model ozone predictions caused by computer simulations of multiple-day periods?

To this point, the discussion of sensitivity analyses has focused on airshed model simulations of one day or less. As we point out in the main body of this report, a reliance on single-day simulations as a means of revealing model sensitivities tends to overstate the importance of air quality data (used to specify initial and boundary conditions, and to understate the importance of other data, i.e., meteorological and emission inputs). Recently, Killus et al. (1980) reported results of a multiple-day simulation for Los Angeles. Using this simulation as a basis for comparison, Souten et al. (1980) conducted a sensitivity simulation to examine the influence of a 57 percent reduction in reactive hydrocarbon initial conditions on predicted ozone maxima on the second day of a smog episode. As indicated in table B-7, model ozone calculations were perturbed by no more than 2 ppb on the second day. These preliminary findings suggest that the need for detailed air quality monitoring data may be reduced if it is possible to develop satisfactory multiple-day simulations for a particular urban area. Of course, as the need for air quality data is reduced by use of multiple-day simulations, the need for improved meteorology becomes more pronounced.

b. Studies Focusing on Meteorological Inputs

Sensitivity studies involving meteorological inputs have investigated variations in wind fields, mixing depths, and diffusion rates. For conservative pollutants, it was found that the airshed model predictions are noticeably more sensitive to reductions in wind speed than to increases (Liu et al., 1976). Furthermore, in another study (Anderson et al., 1977), wind speed reductions appeared to have a far smaller effect on secondary pollutant (ozone) concentrations than on primary concentrations. Finally, the effect of including wind shear (vertical variation in wind speed with height) in place of uniform winds was found to be comparable to a 25 percent increase in surface wind speeds (Reynolds et al., 1976).

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* Linear interpolation of ozone concentrations observed at street-side monitors may grossly underpredict the magnitude of an area-wide ozone levels. Other interpolation schemes, for example, based on mass balances or Poisson fitting routines, may provide more realistic estimates (in some cases).

The study by Liu et al. (1976) indicated that model performance may be degraded more by a reduction in the magnitude of an input variable than by an increase in the magnitude of an input. This trend was found to be the case for mixing depths in their study. Moreover, a concurrent reduction in wind speed and direction revealed that a synergism exists between wind speeds and mixing depths (Anderson et al., 1977). Sensitivity analyses in which horizontal turbulent diffusivity was varied from zero to probably an extreme value for the urban atmosphere during smog episodes (~500 m^2/sec) showed only a minor effect on conservative pollutant concentrations. The effect on reactive species would probably be even smaller. However, the effect on ozone levels of varying the vertical diffusivity an order of magnitude (below and above a base case value) was comparable to varying wind speeds by 25 to 50 percent. Also, a decrease in the vertical diffusivity had a more pronounced impact on ozone predictions than an increase in diffusivity.

In short, the sensitivity studies carried out to date indicate that photochemical model predictions are more sensitive to overall reductions in the magnitude of parameters associated with contaminant dilution--wind speed, mixing depth, and diffusivity--than to corresponding increases in the parameters.

This review found only two studies that addressed the impact on model predictions caused by alternative procedures for preparing meteorological inputs, specifically wind fields (Liu et al., 1976; Reynolds et al., 1979). Liu et al. (1976) investigated two procedures:

> Manual preparation of the wind field by smoothing and interpolating measurement data.

> Automatic preparation of the wind field by numerical weighting and smoothing routines.

The studies by Liu et al. involved (1) randomly varying wind speed measurements by 0 or ±1 mph, and (2) randomly varying wind direction measurements by 0 or ±22.5°. Wind measurements so perturbed were used in the manual and automatic wind field preparation processes. Neither type of perturbation had much influence on grid average concentration deviations (about the base case). However, the maximum local deviations (about the base case) were larger, particularly for the case of variable wind direction.

Reynolds et al. (1979) examined the influence on airshed model ozone predictions caused by the use of alternative wind field generation procedures. Three approaches to the prescription of wind field were investigated:

> Use of an interpolation scheme, together with an objective procedure for minimizing wind field divergence aloft.

> Use of a two-dimensional, diagnostic wind model (Liu et al., 1974).

> Use of a three-dimensional, mass consistent, diagnostic wind model (Yocke and Liu, 1978).

Upon examination of the ozone results, Reynolds noted the following:

> Use of interpolated wind fields leads to the greatest bias toward underestimation at the highest concentration levels.

> Compared with the interpolated and three-dimensional wind field simulations, the two-dimensional wind field simulation exhibits a greater tendency toward overestimation for most of the observed concentration range.

> The three-dimensional wind field simulation exhibits less bias (positive or negative) overall than do the other two simulations.

Estimates of model accuracy and precision were derived through computation of the first and second moments of the distribution of residuals (differences between hourly model calculations and observations). The three wind field sensitivity runs produced these results for ozone and NO_2:

Simulation	Ozone (pphm)		NO_2 (pphm)	
	Accuracy	Precision	Accuracy	Precision
Interpolated wind field inputs	-0.7	6.8	-2.0	3.5
Two-dimensional model wind field inputs	1.4	8.6	-1.5	4.0
Three-dimensional model wind field inputs	0.3	7.6	-2.2	3.7

Reynolds et al. concluded that, on the basis of computed measures of accuracy, precision, and bias, and of precision at upper percentile ozone concentration levels, the three-dimensional wind model appears to offer the best simulation results. However, there were several instances where this procedure for supplying wind inputs led to poorer model performance, such as at a particular monitoring station or over a particular range of observed concentrations.

With the exception of the two studies just discussed, all of the sensitivity studies to date have been designed so that the perturbation to diffusivities or wind fields is uniform across the modeling grid. The same is true for studies involving mixing depths. With the results of past sensitivity studies as a foundation, certain additional analyses might be performed to investigate

> The impact on model predictions of using a fully three-dimensional wind field rather than a uniform field (x,y variations only) or a uniform field "extended aloft", based on theoretical arguments.

> The impact on model predictions caused by horizontal variability in the vertical diffusivity fields.

In the first case, the extent to which model predictions are influenced by the procedure for preparing wind fields will undoubtedly be governed by the meteorological complexity of the urban area whose data base is used in the sensitivity analysis. Model predictions might be much more sensitive to wind field preparation procedures used in a Los Angeles application, for example, than in Tulsa, Oklahoma. Similarly, the horizontal variability in vertical diffusivity is greater over an urban area exhibiting irregular or complex topography than over smooth terrain.

c. Studies Focusing on Chemistry Inputs

Sensitivity studies on the kinetic mechanisms of photochemical models have centered on variations in ambient temperature, relative humidity, and solar radiation. The first two parameters have been shown to be relatively uninfluential in affecting model predictions, at least for the ranges in each variable that were explored (MacCracken and Sauter, 1975). In contrast, variations in solar radiation, which affect the photolysis rates of NO_2, aldehydes, HNO_2, and H_2O_2, have been shown to be quite significant. For example, MacCracken and Sauter (1975) found that a 50 percent reduction in light intensity reduced the peak ozone concentration by 70 percent.

Other possible sensitivity studies involving AQSM kinetic mechanisms could be entertained that might comprise an examination of the effects of

> Attenuating the intensity of solar radiation with height instead of assuming uniform values throughout the depth of the modeling region.

> Prescribing the individual photolysis rates for NO_2, aldehydes, HNO_2, and H_2O_2, instead of assuming that the photolysis rates of the last three species are proportional to the nitrogen dioxide photolysis rate.

> Evaluation of alternative kinetic mechanism such as those proposed by Falls and Seinfeld (1978), Durbin and Hecht (1975), or Whitten and Hogo (1977).

Clearly other sensitivity studies focusing on chemistry inputs can be envisioned, (e.g., to vary chemical reaction rate constants). However, these are perhaps best reserved for the more complex photochemical smog chamber simulations (Whitten and Hogo, 1977) in which explicit rather than condensed mechanisms are used.

d. Studies Focusing on Emissions Inputs

Several basic sensitivity studies have been performed with source emissions:

> Overall increases or decreases in emission rates.

> Relaxation of the spatial resolution of the emission inventory to accommodate a coarser airshed grid.

> Examination of the impact of single point sources or individual source categories on basin-wide oxidant or sulfate levels.

> Localized reductions in emissions with proportional increases elsewhere in the region to give overall emission rates equal to those in the base case.

These first three sensitivity analyses are quite straightforward. As indicated in table B-7, studies involving small overall emission increases or reductions, aggregation of sources into a slightly larger grid, and examination of the influence of minor sources on basin-wide air quality have found that the impact on basin-wide model predictions is relatively small.

One sensitivity analysis performed by Anderson et al. (1977) focused on the influence of spatial variations in emission rates. They found that a reduction in emissions of 25 percent in any one of eight satellite Denver suburbs did not influence the time, location, or magnitude of the region-wide maximum ozone concentration. (In each scenario, no more than 7 percent of the region-wide emissions were redistributed.)

e. Studies Focusing on Grid Specification

DeMandel et al. (1979) report several interesting sensitivity studies that use the LIRAQ model developed at Lawrence Livermore National Laboratory. One evaluation reduced the model's horizontal resolution from 5 km to 10 km. In the single-day simulation, peak calculated ozone levels were reduced 10 percent from 0.20 ppm to 0.18 ppm. This reduction was explained on the basis of "spatial smoothing". The emission densities of precursor species were reduced by spatial averaging over the larger grid cell size. This resulted in lower concentrations of precursors and lower reaction rates.

Reynolds et al. (1979) compared airshed model ozone predictions based on grid resolutions of 2 miles (3.2 km) and 4 miles (6.4 km). Comparison of the temporal ozone profiles at the monitoring stations indicated that, for the most part, the profiles do not change appreciably when the 4 x 4 mile simulation is introduced. Four exceptions were the Reseda, Upland, Azusa, and Pasadena stations. Examination of the profiles indicates that reducing the grid resolution to 4 x 4 miles leads to:

> An increase in predicted concentrations of ozone at Reseda by a few pphm and a broadening of the temporal profile.

> A reduction of the predicted peak ozone level at Upland by roughly 5 pphm.

> A reduction in the predicted peak ozone level at Azusa by about 6 pphm.

> A reduction in the predicted peak ozone level at Pasadena by about 10 pphm.

Reynolds et al. concluded that a decrease in grid resolution may lead to a slight reduction in peak predicted concentrations, at least at certain monitoring stations. Furthermore, the 4 x 4 mile grid run yielded results that were more "accurate" over the entire concentration range, though at peak concentration levels it was less accurate than was the 2 x 2 mile grid simulation.

The studies just discussed represent an important but preliminary step in understanding the sensitivity of photochemical grid models to variations in emissions. While an understanding of the model's sensitivity to overall changes in emissions is naturally of interest, other issues need to be addressed. In the next subsection we consider certain analyses that might be carried out to determine grid model response to various changes in the components of an emission inventory.

5. ISSUES RELATED TO THE PREPARATION OF EMISSION INVENTORIES

Air quality models are generally used in two ways: model performance evaluation and application. Model evaluation consists of tests of the model using a data set or sets to determine the extent to which the model replicates field measurements. One of the objectives of the evaluation phase is to ascertain whether biases exist in the model performance that might later be alleviated by a more suitable treatment of atmospheric processes, alternative numerical methods, more accurate and detailed model inputs, and so on. In evaluative studies, the disaggregation of various sources in an emission inventory by source type is seldom necessary. What is required is overall grid volume emission rates for each pollutant species. Ideally, the temporal distribution of emission rates within each cell is known or inferred from demographic, industrial, commercial, and other types of data.

In contrast, in an applications study, a model is typically used with an assumed set of "worst case" meteorological conditions in conjunction with an emission inventory that reflects a proposed or anticipated change in emissions from some baseline level. If the reduction (or increase) in emissions is uniform, regardless of whether the concern is region-wide or within a given subarea, the emission inventory used for model performance evaluation may suffice. However, if the applications study focuses on the effectiveness of a particular emission control tactic in maintaining or reaching a particular air quality goal, then a more detailed emission inventory may be essential. In the following paragraphs typical emission control measures are identified together with the corresponding level of detail required of an emission inventory so that a complex model could be used to assess the effectiveness of the measure.

To provide a structure for this discussion, table B-8 presents various emission control measures and strategies,* which were selected by the San Francisco Association of Bay Area Governments (ABAG, 1977) from

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* A control measure is an individual emission reduction proposal; a control strategy may entail two or more control measures.

TABLE B-8. CONTROL MEASURES AND EMISSION INVENTORY DATA NEEDS

Control Measure	Data Needs in the Source Emission Inventory
Stationary source measures	
Restrictions on the type of industrial solvents used	Location, size, and operating characteristics* of coating facilities
Closed organic storage	Location, size, and storage characteristics of facilities handling organic chemicals and fuels
Limitation on the maximum SO_2 emissions of any source to a prescribed level	Location, size, and operating characteristics of all SO_2 emission sources larger than a prescribed level
Limitation on the maximum sulfur content in fuel	Location, size, and operating characteristics of combustion sources operating on high sulfur fuel; emission rates given a switch to low sulfur fuel
Best available control technology on new or existing sources	Location, size, and operating characteristics of new or existing sources
New source review with or without offset	Location, size, and operating characteristics of new source as well as the existing source(s) to which the offset is to be applied
Reduction in motor gasoline vapor pressure	Location, size, and operating characteristics of all facilities handling significant quantities of gasoline (see also mobile source emissions measures)

* Operating characteristics of a particular emission source may include such factors as nominal pollutant emission rate, emissions composition, heat flux, elevation of point of emissions, flow rate, diurnal and seasonal variations in emission rates, composition of fuel, and so on.

TABLE B-8 (Continued)

Control Measures	Data Needs in the Source Emission Inventory
NO_x control of off-highway construction and agricultural activities	Temporal and spatial description of construction and agricultural activities (e.g., crop burning) and characterization of emission rates
NO_x limitations on new boilers and furnaces	Location, size, and operating characteristics of new boilers and furnaces
Mobile source emission measures	
Exhaust emission controls	Gridded vehicular emission rates embodying: Spatially and temporally resolved traffic flow characteristics, such as traffic volume, overall driving speed, cruise speed(s), acceleration and deceleration range, percentages of time spent at cruise and at idle, number of speed changes per mile, number of cold starts, etc. Vehicle mix (including age distribution of vehicle population) and model split (between motor vehicles and busses, trains, rapid transit, etc.) Emissions factors based on elevation, the "average vehicle in the region," EPA heavy duty vehicle emission estimates, unique terrain features (grades), etc.
Evaporative emission controls	Gridded estimates of the distribution of "hot soaks" (see reduction in motor gasoline vapor pressure measures)

TABLE B-8 (Concluded)

Control Measures	Data Needs in the Source Emission Inventory
Operation of a retrofit program	Identification of the age distribution of the regional vehicle population and emission rates resulting from evaporative emissions and catalytic exhaust emission retrofit devices
Emission standards for other mobile sources	Emission rates embodying spatial and temporal resolution for mobile sources, including motorcycles, agricultural equipment, construction equipment, vessels, locomotives, aircraft, recreational vehicles, and miscellaneous utility engines (log splitters, tree cutters, etc.)
Motor vehicle inspection and maintenance programs	Estimate of number of vehicles inspected annually and percentage emission reduction attributable to vehicle maintenance, replacement, etc.
Transportation control measures	
Improvement in traffic flow (e.g., ramp metering)	Similar to those under exhaust emissions controls; in addition, estimates of modal shifts and changes in VMT due to the control measure
Reduction of peak-period traffic volumes	Temporal and spatial resolution of trip origins and destinations
Control over auto use and access (e.g., parking limitations, gas rationing, tolls)	Similar to improvement of traffic flow measures above
Encouragement of alternative travel modes (ride sharing, bicycling, etc.)	Similar to improvement of traffic flow measures above

proposals that might be adopted for controlling emissions from stationary, mobile, and land use sources. Though not exhaustive, the measures do reflect a range of possible control methods that might be investigated using air quality models in future SIP analyses.

Considering stationary source control measures first, table B-8 reveals that, for adequate testing of many of the measures, disaggregation of stationary sources by type and size of operation is necessary. Clearly, if one were attempting to assess the impact of controls imposed on dry cleaners, for example, on basin-wide oxidant levels, it would be necessary to locate and define the emission strengths of these numerous sources throughout the urban area. Such a level of detail typically does not exist in most conventional emission inventories. Controls on refinery operations might be easier to analyze given an aggregated emission inventory because of the far fewer number of sources in an urban area and, perhaps, because of a better estimation of overall refinery emission rates. (Note, however, that the distribution of reactive hydrocarbon emissions from refineries is probably poorly known because of numerous fugitive sources and hydrocarbon species.)

Measures that attempt to reduce vehicular emissions are broadly categorized in table B-8 under the headings "mobile source emission measures" and "transportation control measures." Examples of control measures in these categories include

> Stringent exhaust and evaporative emission controls

> Inspection, maintenance, and retrofit programs

> Ramp metering

> Parking limitations and regulations

> Gas rationing

> Increased gas and parking taxes

> "Smog charges"

> Fare reductions on public transit

> Bus and carpool lanes

> Auto-free zones.

As with stationary sources, an analysis of these or other vehicular emission control measures is complicated by the aggregation that takes place in preparing conventional inventories of the emission rates from various sources into a composite value. The processes by which this confounding takes place is summarized next and then suggestions are offered as to how the loss of detailed information on particular sources might be avoided in the preparation of new inventories.

a. Mobile Source Emission Inventories

Three general procedures are used in compiling mobile source emission inventories:

> Manual link-by-link summation

> Automated link-by-link summation

> Estimation based on gasoline sales.

The first method, a tedious one, requires estimation of emissions from each section of freeway and arterial streets on the basis of traffic counts (available on maps from local agencies), peak and off-peak speeds, light versus heavy duty vehicle mix, and "minor" street traffic volumes. Corridor inventories are generated through these analysis; regional inventories are derived by apportioning the corridor emissions to a regional grid and assuming that minor streets contribute some fraction of the corridor emissions.

Automated link-by-link emission inventories are based on regional transportation models. The transportation forecasting model is used to simulate trip generation, travel on various roadway segments, peak and off-peak speeds, total VMT, cold starts, hot soaks, and so forth. These estimates, when combined with appropriate emission factors [such as those contained in AP-42 (EPA, 1972) and the most recent supplements], are used to generate emission rates that are then "loaded" onto a regional emission grid. More flexible than the previous method, the automated approach (which uses a simulation model for traffic characteristics) sacrifices some accuracy by using the transportation model to calculate VMT rather than using actual data.

Finally, gross attempts to construct a regional mobile source inventory can be based on an inventory of regional gasoline sales. Lacking temporal and spatial resolution, this procedure is the least desirable of the three.

Regardless of which of the three basic methods is employed, some details of the vehicular operations (and their spatial and temporal variabilities) that lead to emissions are lost when preparing a gridded regional inventory. Fortunately, in some cases, information concerning vehicle mix, temporal distributions, and so forth can be retrieved. For example, if a modal shift was anticipated because of a particular control strategy, one could go back through the calculations of a manually prepared inventory and apply different light versus heavy duty vehicle mix ratios. Less tedious, with an automated transportation forecasting model, one could change model split factors and rerun the computer code, generating a new set of traffic estimates, which could then be used to revise the mobile source emission inventory.

b. Stationary Source Emission Inventories

This component of the overall inventory consists of major point sources (refineries, smelters, power plants, and so on) and "other" sources. The first category generally does not represent a major problem in constructing an inventory because the main sources are usually easily identifiable. However, frequently the emission characterization of major point sources is made on an annual or "nominal" basis and thus may depart substantially from actual day-to-day emission rates.

Lumped into the "other" source categories are facilities such as cleaners, gas stations, residential chimneys, coating and manufacturing industries, and so forth. Aggregation of these sources into a regional inventory is often considerable. For example, rather than identifying the location and size of each dry cleaner in an urban area, because of time and resource constraints, the inventory may be prepared by (1) determining the total number of dry cleaners in the area (perhaps from the telephone directory), (2) estimating an average perchloroethylene rate for a typical dry cleaning shop (see EPA, 1972), and (3) apportioning the total emissions on a regional grid according to a demographic distribution. While this procedure may be satisfactory from the model verification point of view, it is not acceptable if one is interested in examining the reduction in basin-wide oxidant levels caused in part by controls on evaporative emission sources that include dry cleaners.

Several conclusions can be drawn from the foregoing discussions and the review of previous model sensitivity studies:

> Although the emission inputs required to operate a complex model are relatively straightforward (i.e., gridded emission fluxes of each pollutant), procedures for compiling these inputs exhibit wide variability, ranging

from sophisticated traffic forecasting models to simple estimates based on regional fuel sales.

> In general, emission inventories destined for use in control strategy evaluation must exhibit a greater degree of detail and disaggregation of the various source types than an inventory used in model verification.

> Existing emission inventories do not permit (without additional modification) the evaluation of many possible emission control measures and strategies; only rather general analyses (such as overall emission reductions or modifications of large, stationary sources) are readily facilitated with current inventories.

> In the modification of existing, or the preparation of new, emission inventories, consideration should be given to the range of emission control strategies that are most promising for the region of interest; in so doing, the particular source types amenable to control can be inventoried separately, thereby establishing a basis for future control strategy evaluation.

> Owing to the wide range in methods used to estimate stationary source emission rates and to develop traffic volumes (and hence mobile source emission rates), it is difficult to estimate the costs entailed in enhancing the level of detail in emission inventories. Accurate estimates of the costs required to improve an inventory for a given city can be made only after an examination of the distribution of source types and the procedures used in forecasting traffic volumes.

6. CONCLUSIONS

This appendix presents a broad overview of the range in data input requirements of present generation photochemical grid models. The SAI Urban Airshed Model has been used as the prototype for this discussion. Review of the monitoring and data acquisition activities at various urban areas in the United States reveals a rather broad range in the quality and quantity of the data collected. Only a very cursory attempt has been made to estimate costs of data acquisition because of (1) the wide geographical differences in the cost of such activities, and (2) the rapid rate at which inflation is presently increasing the cost of these activities.

Several model sensitivity studies have been performed in the last few years. In the main, studies involving the Lawrence Livermore National Laboratory's LIRAQ model and the Airshed Model have been the only ones reported in the open literature. Most, but not all, studies have involved uniform reduction or increase in the magnitude of a model input. Only recently have sensitivity studies been performed that address the impact on model calculation caused by the selection of alternative procedures for preparing model inputs.

REFERENCES

ABAG (1977), "Candidate Control Measures," Air Quality Maintenance Plan, Technical Memo 5, Association of Bay Area Governments, Berkeley, California.

Ames, J., et al. (1978), "The User's Manual for the SAI Airshed Model," EPA-68-02-2429, Systems Applications, Incorporated, San Rafael, California.

Anderson, G. E., et al. (1977), "Air Quality in the Denver Metropolitan Region: 1974-2000," EPA-908/1-77-002, Systems Applications, Incorporated, San Rafael, California.

Attaway, L. D., et al. (1976), "Maintenance Shutdown of Tail Gas Treating Unit: An Assessment of Potential SO_2 Concentrations and Related Health and Welfare Effects," TR-11700, Greenfield, Attaway & Tyler, Incorporated, San Rafael, California, and Systems Applications, Incorporated, San Rafael, California.

DeMandel, R. E., et al. (1979), "LIRAQ Sensitivity REsults", Bay Area Air Quality Management District, San Francisco, California.

Demerjian, K. L. (1976), "Photochemical Air Quality Simulation Modeling: Current Status and Future Prospects," Paper 16-1, International Conference on Photochemical Oxidant Pollution and Its Control, Environmental Protection Agency, Raleigh, North Carolina.

Durbin, Paul, and T. A. Hecht (1975), "The Photochemistry of Smog Formation," Internal Paper, Systems Applications, Incorporated, San Rafael, California.

EPA (1972), "Compilation of Air Pollutant Emission Factors," AP-42, U. S. Environmental Protection Agency, Research Triangle Park, North Carolina.

Falls, A. H., and J. H. Seinfeld (1978), "Continued Development of a Kinetic Mechanism for Photochemical Smog: Environ. Sci. Technol., Vol. 12, No. 13.

Hecht, T. A., J. H. Seinfeld, and M. C. Dodge (1974), "Further Development of a Generalized Kinetic Mechanism for Photochemical Smog," Environ. Sci. Technol., Vol. 8, p. 327.

Hickey, H. R., W. D. Rowe, and F. Skinner (1971), "A Cost Model for Air Quality Monitoring Systems," J. Air Pollut. Control. Assoc., Vol. 21, No. 11, pp. 689-693.

Liu, M. K., et al. (1976), "Continued Research in Mesoscale Air Pollution Simulation Modeling: Volume I--Analysis of Model Validity and Sensitivity and Assessment of Prior Evaluation Studies," EPA-600/4-76-016a, Systems Applications, Incorporated, San Rafael, California.

Liu, M. K., et al. (1974), "Assessment of the Feasibility of Modeling Wind Fields Relevant to the Spread of Brush Fires," Systems Applications, Incorporated, R74-15, San Rafael, California.

MacCracken, M. C., and G. D. Sauter, eds. (1975), "Development of an Air Pollution Model for the San Francisco Bay Area," University of California, Livermore, California.

Miedema, A. K., et al. (1973), "Cost of Monitoring Air Quality in the United States," EPA-450/3-74-029, Research Triangle Institute, Research Triangle Park, North Carolina.

Reynolds, S. D., et al. (1979), "Photochemical Modeling of Transportation Control Strategies," report to Federal Highway Administration, EF79-37, Systems Applications, Incorporated, San Rafael, California.

Reynolds, S. D., et al. (1976), "Continued Development and Validation of a Second Generation Photochemical Air Quality Simulation Model: Volume II--Refinements in the Treatment of Chemistry, Meteorology, and Numerical Integration Procedures," EF75-24R, EPA-600/4-26-016b, Systems Applications, Incorporated, San Rafael, California.

Souten, D. R., T. W.Tesche, and W. R. Oliver (1980), "Evaluation of the Air Quality Impacts of Alternative Air Pollution Control Policies Utilizing the Airshed Grid Modeling Approach for the South Coast Air Basin," 305-EF80-220, Systems Applications, Incorporated, San Rafael, California.

Whitten, G. Z., and H. Hogo (1977), "Mathematical Modeling of Simulated Photochemical Smog," EPA-600/3-77-011, Systems Applications, Incorporated, San Rafael, California.

Yocke, M. A., and M. K. Liu (1978), "Modeling Wind Distributions over Complex Terrain," EPA-68-03-2446, SAI No. EF78-78, Systems Applications, Incorporated, San Rafael, California.

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Report identifies key inputs to a photochemical grid model (Urban Airshed Model). A literature review summarizing sensitivity tests performed prior to 1981 is also presented. Costs associated with obtaining various kinds of input data in past studies are also estimated.

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