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UCRL 51660

**DEVELOPMENT OF AN AIR POLLUTION MODEL
FOR THE SAN FRANCISCO BAY AREA**

**Third Semiannual Report
to the
National Science Foundation**

September 23, 1974

Prepared for U.S. Atomic Energy Commission under contract No. W-7405-Eng-48

**LAWRENCE
LIVERMORE
LABORATORY**

University of California/Livermore

MASTER

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Printed in the United States of America
Available from

National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

Price: Printed Copy \$ *, Microfiche \$1.45

<u>* Pages</u>	<u>NTIS Selling Price</u>
1-50	\$4.00
51-150	\$5.45
151-325	\$7.60
326-500	\$10.60
501-1000	\$13.60

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Foreword

This report has been prepared to fulfill the semi-annual report requirement of the agreement between the National Science Foundation and the Lawrence Livermore Laboratory (AG-412), the NASA Ames Research Center (AG-411), and the Bay Area Air Pollution Control District (GI-36390).

This research effort, of wide scope, has been divided into a number of subtasks which are described separately in this report. The project, however, represents a joint effort by the three agencies. On a project of this type, a considerable amount of coordination and cooperation is required among the participants. To separately identify efforts and give proper credit to all the other participants would be both redundant and tedious, and hence no such credit has been cited. The work reported here should be considered the collective effort of all those listed below.

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INTRODUCTION

Through its Research Applied to National Needs (RANN) program, the National Science Foundation is seeking to focus application of this country's vast scientific base to current practical problems of national interest. Under the RANN program, an interagency effort is underway at the University of California Lawrence Livermore Laboratory (LLL), the NASA-Ames Research Center (ARC) and the Bay Area Air Pollution Control District (BAAPCD) to develop and validate a regional air pollution model which can be applied to the air quality problems facing the San Francisco Bay Area. Previous Semi-annual Reports (UCID-16301, July 9, 1973; UCRL-51537, February 27, 1974) reported on the organization of the development project, progress made, and plans for the remaining time.

As reported earlier, the planned research activities were divided into five major subtasks, and a joint working group was established for each - Operational Planning, Source Inventory, Photochemistry, Model Development and Validation, and Model Applications. Each joint working group includes representatives from each of the three agencies.

OPERATIONAL PLANNING GROUP

This group has responsibility for choosing instrumentation, selecting observation techniques, planning aircraft schedules and flight paths, coordinating and gathering ground station data, archiving data, developing a usable data storage system, and providing data for model validation.

SOURCE INVENTORY GROUP

This group has responsibility for providing a time - and space - varying source inventory for

both mobile and stationary sources and for the appropriate selection of pollutants.

PHOTOCHEMISTRY GROUP

This group has responsibility for developing appropriate reaction and pollutant sets, assessing mathematical solution methods, comparing model results with smog chamber results, and establishing criteria for characterizing the reactivity of the various source emissions.

MODEL DEVELOPMENT AND VALIDATION GROUP

This group has responsibility for model development covering aspects of topography, meteorological data, transport and photochemistry, and also for model validation and later application.

MODEL APPLICATION GROUP

This group has responsibility for setting goals for model use, determining the practical limits for model accuracy and resolution, and for proposing validation and perturbation studies to determine model suitability.

MANAGEMENT OVERVIEW

In addition to the frequent interfaces resulting from group committee activities, bimonthly review meetings are held among the principal investigators, the Program Director, and other investigators. The objectives of these meetings are to review progress and to address possible problems that transcend the responsibility and capability of any single working group.

ASSESSMENT OF PROGRESS

As of July 1, 1974, the various activities were proceeding on schedule. As reported in the second semi-annual report, Aircraft Flight Data from the 1973 sampling flights have been manually reduced and prepared for entry into the data bank. Data from 1974 flights should become available by fall, 1974, at which time extensive model validation will begin. Development of the various submodels is on schedule and increasing effort is now being expended to develop graphical display of model results.

Stationary source emission data are entered into the data bank and updated as new data become available.

Effort to develop a comprehensive mobile source emission inventory continues and should be available to the model by October 1974.

Plans are complete to conduct fluorescent particle tracer experiments to investigate transport between the inversion layer and the mixing layer. Initial experiments are planned to start in August, 1974.

A first set of reduced photochemical reactions has been selected and work will continue to assess assumptions and to test the sensitivity of the reactions to various parameters. The reduced set will be included in test runs of LIRAQ-2 in late summer.

SUMMARY OF ACTIVITIES

OPERATIONAL PLANNING

Field operational activities during the summer and fall of 1974 were discussed at a meeting of the Operational Planning Group at San Jose State University on 2 May 1974. We agreed that the plan of operations would remain essentially unchanged from that used in 1973. The NASA aircraft will fly approximately 200 hr of sampling runs on suitable days to be selected by the BAAPCD. The concept of "planning windows" used in 1973 will be abandoned this year in favor of a more flexible system consisting of an alert 48-hr before an operation and a "go" or "no-go" decision 24 hr in advance. A dry run of a complete operation (including the preparation of an in-flight test of the NASA airborne data acquisition system) was scheduled for late June. Recording of data from the aircraft INS system will not be possible until about mid-June. The first actual flight operations are tentatively scheduled for July.

A specialized fluorescent tracer experiment will be conducted this year to investigate the nature of transport through the inversion layer. Arrangements have been made with Metronics Associates of Palo Alto, California to perform the experiment. Five operations under suitable conditions are planned, including:

(1 & 2) Tracer release at midday in the Hayward area, one in and one above the inversion layer. These operations will be conducted under conditions of transport between the east bay and the Livermore Valley to investigate the extent to which air in the inversion layer is entrained in the mixing layer under conditions of flow across the east bay hills, and the gradient of inversion base heights from the east bay to the valley.

(3) A tracer release in the morning above the inversion base in the Livermore Valley. This operation will be conducted under conditions of light winds and strong insolation to investigate fumigation of inversion layer pollutants as the inversion layer is eroded by surface heating.

(4) A tracer release in the evening, south of San Jose, under prolonged conditions of stagnation to investigate the recirculation of pollutants, and,

(5) A tracer release under conditions yet to be determined.

All releases will be made from a helicopter using two aerosol generators. All tracer sampling will be done with two Mee airborne real-time samplers mounted on two fixed-wing light aircraft. BAAPCD is responsible for the overall operational planning associated with this experiment.

SOURCE INVENTORY

Stationary Sources

The stationary source inventory is complete and is being updated as new information becomes available. The contaminants contained in the stationary source inventory are particulates, organics, oxides of sulfur, nitrogen oxides, and carbon monoxide. The inventory is maintained in terms of emissions per 1-km grid square defined in Universal Transverse Mercator (UTM) coordinates.

The stationary sources include the 98 major industrial sources for which the BAAPCD has published data on average daily emissions. In addition, nonindustrial stationary sources (e.g., home heating) have been distributed geographically, based on demographic information obtained from the U.S. Census Bureau through the Association of Bay Area Governments (ABAG). Detailed information concerning stack height, operating schedules, and other data are being gathered and entered into the data base as they become available.

Aircraft emissions data are being prepared for distribution on the grid and inclusion in the data bank. The meager data on the composition of jet fuels have required the development of gas chromatographic techniques for the analysis of jet fuels. Resolution of JP-4 and JP-5 reveals that JP-4 contains a significant fraction of C_8 and C_9 hydrocarbons that are absent in JP-5. By the use of selective scrubber columns, a separation of the fuel into aromatic-olefin, straight-chain, and branched-chain hydrocarbon fractions should be possible. Upon completion of this fuel analysis we expect to be able to assign reactive indices to the three hydrocarbon types present in jet fuel. This will be necessary to estimate the pollutant contribution of jet fuel from evaporation and ground operations at the airports of the Bay Area.

Mobile Sources

Data on vehicular emissions are based on traffic information obtained from the Metropolitan

Transportation Commission (MTC) of the San Francisco Bay Area and the California Division of Highways (CDH). The results of a regional traffic model for 1965 were supplemented by 1972 ground traffic counts conducted by the CDH. The CDH traffic counts and other statistical data were used to adjust the traffic model data provided by the MTC. These calculations provided a first set of mobile source emissions data.

The model for the mobile source inventory must consider temporal variations as well as spatial resolution. In addition, emission factors corresponding to the mixture of vehicles in the region must be determined. To aid in calculating these data, a subcontract has been awarded for the development of procedures, performance of calculations, and the delivery of data for 1973 and 1980 vehicle emission estimates.

Due to a delay in obtaining 1980 data from MTC, the scheduled completion has slipped from April to September, 1974. Significant progress toward developing a comprehensive mobile source inventory has been made, however, as seen in the status of the following tasks:

(1) Update of 1973 network has been completed. Evaluation of 1973 network by the MTC staff has been conducted, and speed corrections and other comments provided by the MTC staff have been incorporated in the final network update.

(2) 1980 network and trip-end data were provided by the MTC in mid-May. Several test runs for trip distribution and assignment models have been conducted. The final travel pattern model (trip distribution and assignment) is complete.

(3) Truck trip and external trip data were obtained from the MTC and California Department of Transportation. Data were analyzed and compiled as input format for 1973 and 1980 trip tables.

(4) Temporal and spatial distribution of average daily traffic for the Bay Area were delineated and analyzed from various data sources.

(5) Analyses and evaluation of various emission factors for mobile sources were conducted. Emission factors developed by BAAPCD with EPA speed correction factors were selected for use in the project.

PHOTOCHEMICAL KINETIC MODELS

A photochemical reaction set for initial testing in the LIRAQ-2 model has been selected, although some further sensitivity testing, tuning, and assessment of the steady-state assumptions must be undertaken. The mechanism will use the reactions of Table 1, and the inorganic rate coefficients will be taken from the NBS recommendations (NBSIR-74-430). The organic reactions are based on a lumping scheme.

Organics are lumped into three classes based on their reactivities toward ozone and sunlight. These are: HC_1 - reacts with O , OH , O_3 (olefins); HC_2 - reacts with O , OH (alkanes, simple aromatics, ethers, alcohols, etc.); and HC_3 - reacts with O , OH , sunlight (aldehydes, some ketones, and some aromatics). Because these classes of hydrocarbons do not refer to individual chemical species or their daughter compounds, all reactions involving organic species are parameterized based on the detailed inventory of hydrocarbons and the temporal emissions pattern.

In order to reduce the mathematical "stiffness" of the set and the number of species to be followed, some ap-

proximations have had to be made. First, some species enter the scheme only as products. Unless they are of particular interest they will not be followed further. These include PAN, RNO_3 and CO_2 . Some species are either constant in concentration (O_2 , $ZM \equiv N_2 + O_2 + H_2O$) or are present at concentrations almost unaffected by photochemistry. These species will be prescribed by transport and meteorology: H_2O , CO . In addition, the light intensity and the surface loading of aerosol (A_s) will be prescribed. Further, the following species will be treated via a stationary state approximation: O , NO_3 , HO , HO_2 , RO , RO_2 , RCO_3 .

This leaves the following species to be treated interactively: NO , NO_2 , N_2O_5 , O_3 , H_2O_2 , HC_1 , HC_2 , HC_3 , RNO_2 , $ROOH$, HNO_3 , HNO_2 . The least important species is probably HNO_2 , with $ROOH$ also of limited importance except as a sink. If, say, PAN were to be followed, it might be reasonable to omit reactions 43 and 52 (Table 1) and follow PAN instead of $ROOH$.

Table 1. Photochemical reaction set

Reaction Number ^a	k LLL at 25°C
1. $\text{NO}_2 + \text{ZRAD} \rightarrow \text{NO} + \text{O}$	p
2. $\text{O} + \text{O}_2 + \text{ZM} \rightarrow \text{O}_3 + \text{ZM}$	6.06×10^{-34}
3. $\text{O}_3 + \text{NO} \rightarrow \text{O}_2 + \text{NO}_2$	1.52×10^{-14}
4. $\text{O} + \text{NO} + \text{ZM} \rightarrow \text{NO}_2 + \text{ZM}$	9.78×10^{-32}
5. $\text{O} + \text{NO}_2 \rightarrow \text{O}_2 + \text{NO}$	9.1×10^{-12}
6. $\text{O} + \text{NO}_2 + \text{ZM} \rightarrow \text{NO}_3 + \text{ZM}$	5.0×10^{-32}
7. $\text{O}_3 + \text{NO}_2 \rightarrow \text{NO}_3 + \text{O}_2$	4.25×10^{-17}
8. $\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$	3×10^{-12}
9. $\text{N}_2\text{O}_5 \rightarrow \text{NO}_3 + \text{NO}_2$	2.3×10^{-1}
10. $\text{NO}_3 + \text{NO} \rightarrow 2\text{NO}_2$	8.3×10^{-12}
11. $\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2\text{HNO}_3$	6×10^{-21}
16. $\text{HNO}_3 + \text{ZRAD} \rightarrow \text{HO} + \text{HO}$	p
17. $\text{HO} + \text{NO}_2 \rightarrow \text{HNO}_3$	5×10^{-12}
18. $\text{HO} + \text{NO} \rightarrow \text{HNO}_2$	2×10^{-12}
19. $\text{HO} + \text{CO} \rightarrow \text{CO}_2 + \text{HO}_2$	1.33×10^{-13}
20. $\text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}$	1.73×10^{-13}
21. $\text{H}_2\text{O}_2 + \text{ZRAD} \rightarrow 2\text{HO}$	p
22. $\text{HC}_1 + \text{O} \rightarrow \text{RO}_2 + (\alpha)\text{RCO}_3 + (1-\alpha)\text{HO}_2$	4.53×10^{-12a}
23. $\text{HC}_1 + \text{O}_3 \rightarrow \text{RCO}_3 + \text{RO} + \text{HC}_4$	1.07×10^{-17a}
24. $\text{HC}_1 + \text{HO} \rightarrow \text{RO}_2 + \text{HC}_4$	1.7×10^{-11a}
25. $\text{HC}_2 + \text{O} \rightarrow \text{RO}_2 + \text{HO}$	6×10^{-14a}
26. $\text{HC}_2 + \text{HO} \rightarrow \text{RO}_2 + \text{H}_2\text{O}$	3×10^{-12a}
29. $\text{HC}_4 + \text{ZRAD} \rightarrow (\beta)\text{RO}_2 + (2-\beta)\text{HO}_2$	p,a
30. $\text{HC}_4 + \text{HO} \rightarrow (\beta)\text{RCO}_3 + (1-\beta)\text{HO}_2 + \text{H}_2\text{O}$	1.4×10^{-11a}
31. $\text{RO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{RO}$	6.1×10^{-13a}
32. $\text{RCO}_3 + \text{NO} \rightarrow \text{RO}_2 + \text{NO}_2 + \text{CO}_2$	6.1×10^{-13a}
33. $\text{RCO}_3 + \text{NO}_2 \rightarrow \text{PAN}$	6.65×10^{-14a}
34. $\text{RO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{HC}_4$	5×10^{-18a}
35. $\text{RO} + \text{NO}_2 \rightarrow \text{RNO}_3$	3.25×10^{-13a}
36. $\text{RO} + \text{NO} \rightarrow \text{RNO}_2$	1.66×10^{-13a}
37. $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	5.48×10^{-12}
38. $\text{RO}_2 + \text{HO}_2 \rightarrow \text{ROOH} + \text{O}_2$	3×10^{-12a}
39. $\text{RO}_2 + \text{RC}_2 \rightarrow \text{R}_2\text{O}_2 + \text{O}_2$	2×10^{-12a}
40. $\text{HC}_4 + \text{O} \rightarrow (\beta)\text{RCO}_3 + \text{HO} + (1-\beta)\text{HO}_2$	1.6×10^{-13a}
42. $\text{RNO}_2 + \text{ZRAD} \rightarrow \text{RO} + \text{NO}$	p,z
43. $\text{ROOH} + \text{ZRAD} \rightarrow \text{RO} + \text{HO}$	p,a
45. $\text{NO}_3 + \text{ZRAD} \rightarrow \text{HO} + \text{O}_2$	p
46. $\text{HO}_2 + \text{HC}_4 \rightarrow \text{H}_2\text{O}_2 + \text{RCO}_3$	1.33×10^{-17a}
47. $\text{RO}_2 + \text{HC}_4 \rightarrow \text{ROOH} + \text{RCO}_3$	1×10^{-17a}
48. $\text{O}_3 + \text{ZRAD} \rightarrow \text{O} + \text{O}_2$	p
49. $\text{RCO}_2 + \text{NO} \rightarrow \text{HC}_4 + \text{HNO}_2$	2×10^{-13a}
50. $\text{O}_3 + \text{ZRAD} + \text{H}_2\text{O} \rightarrow \text{O}_2 + 2\text{OH}$	p
51. $\text{N}_2\text{O}_5 + \text{ZRAD} \rightarrow \text{NO}_2 + \text{NO}_2 + \text{O}$	p

^a Missing numbers result from reducing list from previous report.

^p photolysis rate is a function of zenith angle, cloud coverage.

^a parametric rate. The values given are untuned parameters based on specific smog chamber studies, and need to be adjusted to fit the atmosphere.

In addition, the following heterogeneous reactions will be used. (A_s stands for aerosol.)

52. $ROOH + A_s \rightarrow A_s$	Diffusion limited
53. $RNO_2 + A_s \rightarrow A_s$	Diffusion limited
54. $HNO_3 + A_s \rightarrow A_s$	Diffusion limited
55. $H_2O_2 + A_s \rightarrow A_s$	Diffusion limited
56. $HNO_2 + A_s \rightarrow A_s$	Diffusion limited

These reactions are sink reactions. The proper treatment of them is the subject of ongoing research. The reactions remove hydrocarbons and NO_x from the system.

Recent modification of the Ames detailed reaction mechanism has led to an upward revision in the value of the rate constants associated with the reaction of hydroxyl and hydroperoxyl radicals with reactive hydrocarbons. These new values now bring $KHO_2 + \text{olefin}$ and $KOH + \text{olefin}$ into good agreement

with the values recommended by Hecht and Seinfeld,¹ Nikl,² and Calvert.³

Numerical analysis of a computer simulation of a two hydrocarbon mixture has demonstrated the possibility of applying steady-state assumptions to NO_3 and all free-radical species other than the oxides of nitrogen. Moreover, H_2O , N_2 , and O_2 are essentially constant and represent the relative humidity of the lower atmosphere.

Based on the contribution of individual reactions to the overall production or destruction of a given species, a total of 21 reactions can probably be deleted from the Ames mechanism. It also appears possible that a reduced reaction set of 45 reactions involving 22 species may be capable of an adequate description of photochemical smog. Work at LLL suggests that the number of species can be reduced to 12. Concurrent development of both reduced sets should permit the validation of a reduced reaction set by August 1974.

MODEL DEVELOPMENT AND VALIDATION

Model development and validation consists of many phases. Overall, the several aspects are intermeshing well, although progress in validation and updating of each part has varied, depending on the availability of data and other factors. More detail is provided by looking at each aspect of the modeling sequence.

Utilization of the Data Base

Data collection efforts during 1973 resulted in 4,824 logical records processed into the Master Control data base, with 3,851 records originating from fixed locations and 973 records from the NASA Ames aircraft. The Ames aircraft data has been available only for the period 26-27 July as it had to be keypunched due to onboard data acquisition system difficulties. Aircraft observations were logged at approximately 1-min intervals rather than 20-sec intervals as originally planned. At 150 mph ground speed and 1-min intervals, data points are approximately 2.5 miles apart. The 20-sec interval is preferable, if feasible, since finer resolution of the data, particularly around urban areas, is desirable. Measurements of the nitrogen oxides, hydrocarbons, and, often, wind speed/wind direction were not available from the Ames aircraft. Wind information is especially desirable since our spatial coverage of the vertical wind structure over the modeling area is sparse. It would allow us to determine where pollutants were being advected from. Further we could examine the validity of using a power law wind profile with a constant direction assumption and

the subsequent application of a mean layer wind as the basic input to the transport aspect of the model.

The Master Control data base has been used in several ways. Data sets over the 26-27 July case study period have been extracted to test the model. In addition, data sets of primary pollutants have been extracted from the data base (using nested searching techniques and macro expansions) in our attempt to verify model output. We are also experimenting with graphical representation of selected data in the form of standard meteorological displays of vertical wind reports, isoline contour analyses in the horizontal, and time-lapse movies of the NASA aircraft information.

Mass Consistent Wind Field Model (MACAW)

The MACAW model is developed, as indicated in the second semi-annual report. Provision is included for inversion height change due to several factors, and preliminary studies for the July 26-27 period indicate that factors other than convergence and divergence are very important. To assess these will require data on air flow through the inversion and quite accurate vertical soundings of wind speed. The early data from the 1973 aircraft flights do not appear adequate to assess this satisfactorily. However, the tracer studies planned for 1974 are expected to be quite useful. As a temporary alternative we are making some rather *ad hoc* choices about the relative importance of the various factors.

Validation procedures for the model are in their early stages. We are now formulating a statistical procedure to assess the changes MACAW makes to the observed wind field in performing the mass consistent adjustment.

Topographic Data

As described in the second semi-annual report, the topographic data handling routines are essentially complete. They have been used to provide the input tape for LIRAQ-1 for topographic, bay area outline, and station location data on a rotated, 7-km grid. The routines are structured to be able to treat different grids depending on the problem of interest, an option we expect to test in the near future.

Source Data

The first phase development of the source data handling routines are quite fully described in the second semi-annual report. This package was used to generate the initial LIRAQ-1 validation studies in January. Some improvements are needed, based on an evaluation of the earlier simulation.

Rather than two basic data files, three basic data files should be formed. These files would contain (1) surface stationary emissions, (2) surface vehicular emissions, and (3) elevated point source emissions. The data in file (1) would include the population-distributed stationary sources plus all major industrial sources that are not emitted at a significant stack height. The data in file (3) would include all elevated major industrial sources plus commercial airport emissions. All data files would be kept in terms of the 1-km UTM grid squares. The data in files (1) and (2) would be used in LIRAQ as is presently done, but the data in file (3) would *not* be used in calculating the surface pollutant concentrations. These elevated emissions should be included as extra sources (i.e., in addition to the surface sources) in solving the transport equation for the mean concentration. This modeling procedure will lessen the impact of strong, elevated point sources on the surface concentrations calculated at the source location.

In order to achieve this assignment of sources, several improvements in the data must be undertaken. Airport emissions, which are currently population distributed, must be removed from this category and assigned to the grid squares where those emissions actually occur. Also, a definition of "significant" stack height consistent with this procedure must be given. Wherever possible, data on the diurnal variation of emissions from the major sources, elevated or not, should be obtained and used rather than relying on *ad hoc* assumptions. The new calculation of vehicular emissions will include intrazonal sources derived from

traffic assigned to "dummy links" which do not cross traffic zones. These intrazonal sources must be distributed to the UTM grid squares in a fashion similar to that used for vehicular sources.

LIRAQ-1 Model

The initial phase of development of the LIRAQ-1 model is complete, as described in the second semi-annual report. Improvements planned in the second phase, including simplified chemistry and improved treatment of the source inventory, are dependent on our model validation studies for the 1973 case days.

Although validation against the 1973 case days has been initially undertaken, a more complete study awaits incorporation of the aircraft data into the meteorological input set for the models.

Studies of the numerical errors made in the differencing approximation of the model will soon be undertaken in conjunction with a graduate student project to convert the model to use flux corrected transport.

LIRAQ-2 Model

Programming of the LIRAQ-2 model is underway and the initial phase work should be completed by late summer. The reaction set described earlier will be incorporated. Initial runs of the model, however, will depend on some updating of the input from the data base to the model to include, for example, temperature and cloudiness information.

MODEL APPLICATION

The primary significance of the NSF model for the work of the BAAQCD will be with respect to: (1) photochemical pollutants, (2) regional-scale analysis, and (3) policy oriented problems. For these applications, the climatological mode of operation is appropriate. Model validation against a climatological mean is a difficult but essential task, and requires a measure of meteorological variability, using Smalley Patterns or simulated wind-flow patterns.

Applications planning emphasizes the importance of statistical measures of confidence intervals associated with model results.

Typical scenarios for both event- and climatological-mode situations have been defined and specified, and running of the model for these scenarios include:

- 1) Determination of minimum emission rate changes in each contaminant of interest to produce a significant change in concentrations.

2) Determination of relative importance of local and imported pollutants in selected areas of the District.

3) Impact on downwind receptor areas of reallocating emissions within a local source area.

4) Distribution of CO concentrations within a local area, using 1-km² resolution.

5) Determination of annual average zone and CO concentrations in selected areas given a known emissions inventory.

6) Determination of annual variability of zone and CO in selected areas as a cumulative probability distribution.

Work has proceeded on the construction of a methodology for selecting the most effective strategy to maximize a given objective function. This will take the form of a model to be used in conjunction with the NSF model for land-use planning purposes, with specific attention to the concept of emissions allocation by geographic subarea. The objective function to be maximized may be defined as the carrying capacity or loading capacity of an area and its subareas in terms of emissions. Actual testing of this methodology will require substantial computational capacity and is in large part beyond the scope of the current project, but this work is important to the BAAQCD for long-range planning applications.

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