EXAMINATION OF REGIONAL PHOTOCHEMICAL MODELS BY A USER

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During 1974 and 1975, there was considerable discussion of the use of regional photochemical models to assess the impact of transportation systems on the air environment. Considerable progress was made to provide operational computer models that can be used by transportation planners and engineers. However, certain issues involving data input requirements and model refinements must be resolved before transportation planners are able to apply photochemical models for planning activities. The purpose of this paper is to discuss, from the user's point of view, the broad application of photochemical modeling, input data requirements, appropriateness of existing data sources, possible solutions to updating air quality data bases, and modeling approaches that are available to solve practical transportation planning problems.

APPLICATIONS OF REGIONAL PHOTOCHEMICAL MODEL FOR TRANSPORTATION PLANNERS AND ENGINEERS

We all recognize that an air model is an essential component of planning studies because of the need to establish a quantitative relation between emissions and their resulting ground-level pollutant concentrations. Every urban area has unique climatological and meteorological conditions. The spatial distribution of emissions, as well as the composition of these emissions, varies from city to city. The concentrations of secondary pollutants, formed in the atmosphere through the chemical reactions of primary (emitted) pollutants, are influenced by local meteorology, emissions patterns, intensity of solar radiation, and many other variables. Clearly, to predict the spatial and temporal distributions of ground-level concentrations of air pollutants requires that account be taken of these many complexities through the simulation of physical and chemical processes that actually give rise to the air quality observed.

A photochemical model can be defined as a mathematical representation of air movements and chemical reaction processes that, when combined with emissions and meteorological data, can be used to predict the temporal and spatial distribution of air pollutants. Air quality models can be used as a "tool" in the decision-making process provided the models have been verified with actual field measurements and quality input data are available. Under these conditions, models can assist transportation planners and engineers to

1. Assess the impact of highways or multimodal transportation systems on air quality;
2. Provide a systematic procedure to evaluate the interrelations of land use, transportation, and air quality;
3. Select the locations for future transportation facilities to minimize the air quality impacts (spatial alternative);
4. Evaluate the impact of transportation control plans;
5. Estimate air quality for areas in which pollutant measurements are unavailable; and

6. Comply with federal and state legislation concerning environmental impact assessment.

MODELING APPROACHES

Air quality models are generally based on the solution of the conservation-of-mass equation. The conservation-of-mass equation for a given air pollutant species and chemical reactions can be expressed as

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x}\left[K_H\frac{\partial c_i}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_H\frac{\partial c_i}{\partial y}\right] + \frac{\partial}{\partial z}\left[K_z\frac{\partial c_i}{\partial z}\right] + R_i + S_i \quad (1)$$

where

c_i = concentration of pollutant species i;
x,y,z = Cartesian coordinates;
u,v,w = wind speed in the x, y, and z directions respectively;
K_H,K_z = horizontal and vertical turbulent diffusivities;
R_i = rate of production of species i through chemical reactions; and
S_i = rate of production of species i from source emissions.

The numerical solution of equation 1 (1) is solved by using either a Eulerian or a Lagrangian coordinate system. The Eulerian coordinate system is fixed to the surface of the earth, and the Lagrangian coordinate system is a moving system. The Eulerian solution is commonly referred to as a grid model, and the Lagrangian solution is referred to as a trajectory model.

In the grid model the study region is divided into a 3-dimensional array of cells (Figure 1). Each cell can vary from 1 to 4 km (0.6 to 2.5 miles) on a side and on the order of 10 to 100 m (33 to 330 ft) high. The size of each cell, of course, will depend on the size of the study area, spatial distributions of emission fluxes of pollutants, terrain affects that may alter the surface winds, and inversions. The solution of equation 1 is achieved by numerically integrating the equation in 3-dimensional space and in time over each grid.

In the trajectory model, a column of air is followed through the study area as it is moved by the surface winds. The air pollutants are emitted into the column as fluxes at the ground surface. As the column passes over the study area, chemical reactions take place within the column.

Existing regional air quality models are capable of predicting the temporal and spatial distribution of concentrations for the following pollutants: carbon monoxide (CO), nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), unreactive hydrocarbons (URH), and reactive hydrocarbons (RHC). The unreactive hydrocarbons are generally taken to be methane, propane, benzene, and acetylene.

Clearly, for each grid square, a description of the temporal and spatial distribution of emissions (both stationary and mobile), meteorological conditions, and initial air quality concentrations must be specified, or calculated from known data. (Only for the initial first hour of simulation must the concentration fields be known or calculated.)

INPUT TO REGIONAL PHOTOCHEMICAL MODELS

A common trait of all regional photochemical models is their need for vast amounts of emissions, meteorological, and air quality data. The greater the quality of the data base is, the better is the ability of the model to simulate events in the atmosphere with

Figure 1. Typical grid study area for Los Angeles.

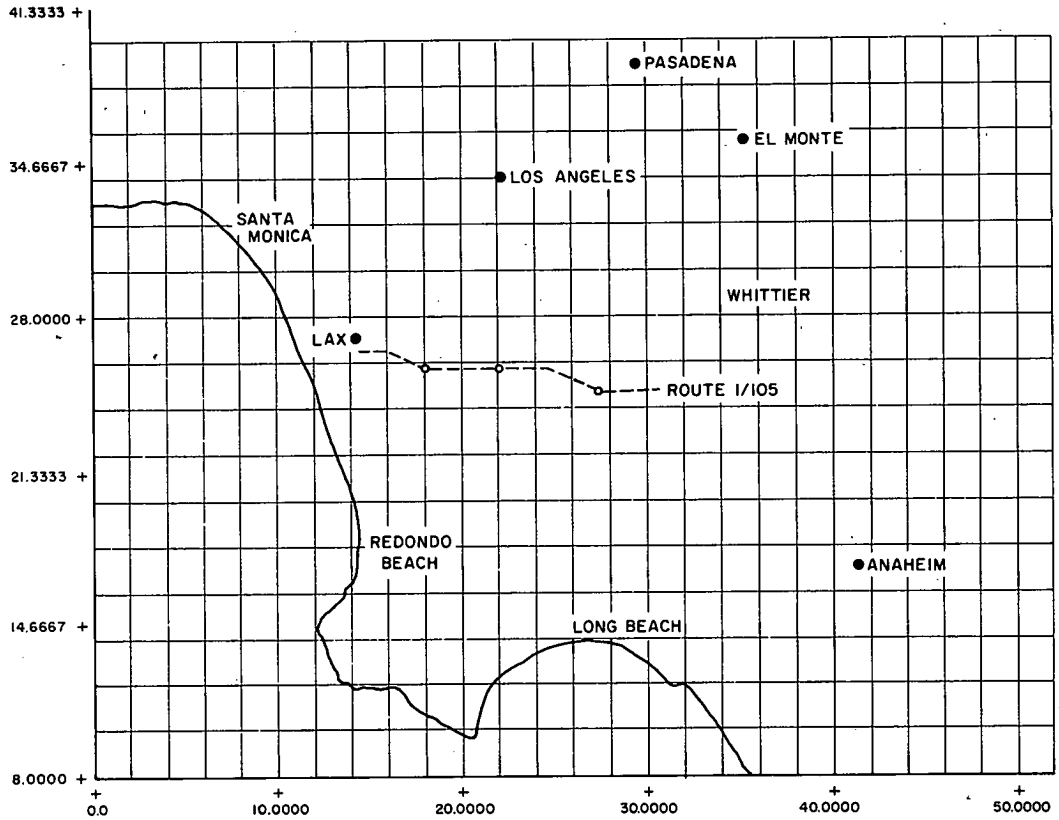
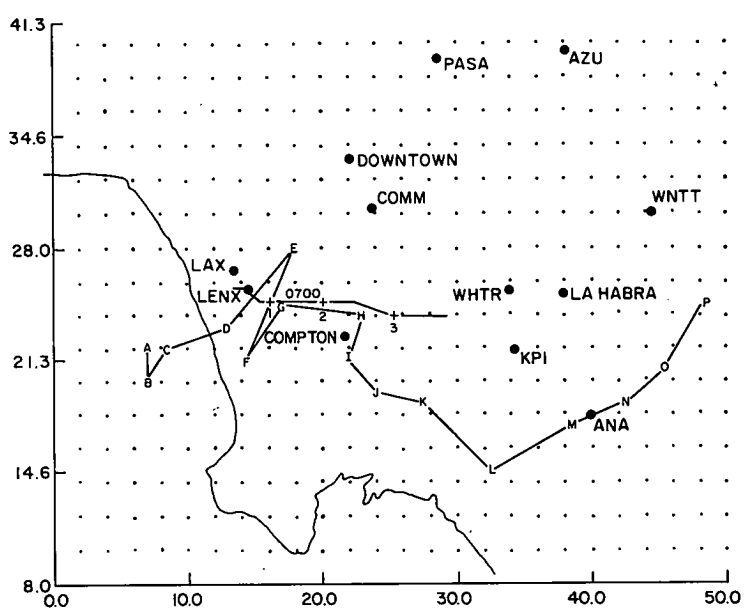


Figure 2. Typical trajectory simulation for Los Angeles area.



a higher degree of confidence. First, the emission inventories (both mobile and stationary sources), meteorology, and the initial hour of air quality data throughout the region are needed so that the model can simulate the transport and diffusion of the emission fluxes while it attempts to duplicate the chemical reactions that occur in the atmosphere. Second, air quality data are required so that air quality predictions can be compared with real-world observations. This verification allows confidence in the model so that it can be used for predicting future pollutant concentrations for air quality impact assessment.

Emission Inventory

The emission inventory must provide estimates, by category, of vehicular, aircraft, power plant, refinery, and distributed area sources including their temporal variations. The emission sources spatially distributed over a grid system (Figure 1) must have a temporal resolution of 1 hour because the air quality standards are generally based on a 1-hour exposure time. For the emission inventory, the following information is required (2). For all of the emission inventories, the ratio of NO to NO_2 is also needed.

Vehicles

Information required for vehicles is

1. Spatial distribution of daily vehicle kilometers traveled (vehicle miles traveled, VMT);
2. Temporal (hourly) distribution of vehicle kilometers traveled;
3. Average emission rates (mass/distance) of CO, NO_x, and HC;
4. Spatial and temporal distributions of average vehicle speed;
5. Variations in emission rates with average speed for CO, NO_x, and HC; and
6. Effects on average emissions rate of cold-start and hot-running operations.

Aircraft

Information required for aircraft is

1. Ground operations emission rates of CO, NO_x, and HC as a function of traffic level, mode of operation, aircraft class or type, location, and time; and
2. Flight operation emission rates as a function of the same variables as those of ground operations emission rates, but segmented into taxi, landing, and takeoff modes.

Power Plants

Power plant information is

1. Emission rates of NO_x for each plant as a function of type of fuel burned, time of day, and time of year;
2. Emission rates of NO_x and organic gases for each refinery; and
3. Emission rates of CO, NO_x, and organic gases for distributed stationary sources as a function of location.

Meteorological Data

The meteorological data, treated entirely as input to the model, in the most comprehensive form include the items listed below:

1. Wind speed and direction, both at the surface and aloft, as a function of location and time;
2. Temperature as a function of height (to permit estimation of stability), location of the inversion layer and inversion base, and strength of the inversion;
3. Vertical turbulent diffusivity as a function of height, ground location, and time of day (this is estimated from various correlations as a function of turbulent energy dissipation rate, wind shear, vertical temperature gradient, wind speed, and surface roughness); and
4. Insolation as a function of ground locations, elevation, and time of day.

Initial Concentration Fields

The air quality data required to establish initial concentration fields at the surface and aloft for a full 3-dimension simulation are concentrations for CO, NO, NO_2, O_3, RHC, and URH. The richness of such a data base described in the above varies within a given region based on the availability of obtaining a complete and up-to-date emission inventory, number of surface air and meteorological monitoring stations and their separation distance, and the frequency of measurements of vertical temperature profiles and wind and air quality data aloft.

PROBLEMS WITH USING EXISTING AIR QUALITY DATA BASES

Many urban areas appear at first glance to have a sufficient emission inventory and an aerometric data base that can be used in photochemical models. This observation is generally based on the number of air monitoring and meteorological stations that exist in a given network. Before making a hasty decision that the inventory is adequate, however, one should be able to answer the following questions.

1. Are the air and meteorological monitoring stations located such that they measure representative data consistent with model assumptions to describe the temporal and spatial distribution of surface winds and air quality?
2. Are the air monitoring networks located near a localized source of pollutant emissions?
3. Is there a standardized height above the ground surface for the entire network from which the air and meteorological measurements are made?
4. Are the recorded hourly values of air quality concentrations and surface wind measurements based on an integrated hourly average or instantaneous reading?
5. How often are the air and meteorological instruments calibrated to provide quality assurance control of the data collected?
6. Are stationary source inventories up to date?
7. Is the vehicular emission inventory based on the latest emission factors published by U.S. Environmental Protection Agency?
8. For the year in question, do transportation simulation models used to estimate vehicle kilometers traveled consider that the price of gasoline has doubled? What effect, if any, has this had on the estimates of vehicle kilometers traveled for the region?

These are just some of the more obvious questions that transportation planners and engineers should consider before using any existing data. If, for the existing data base, satisfactory answers to the questions cannot be evaluated, then the user is confronted with the decision of providing an initial investment to obtain quality inputs. A discussion of the problems is described below.

Definition of Grid Boundaries or Study Region

The first step involved in applying a regional air quality model is to decide on the size

of the study area. Because of the multidisciplinary expertise required to develop inputs for the models, the exact boundaries for an urban area should be coordinated with local land use planning agencies, air pollution control districts, and transportation planners. Major factors to consider in defining the region should include populated areas, areas of high pollutant concentrations, areas of high emissions, topography and terrain features, and local master plans for future developments. All agencies involved must agree to a common region, coordinate system, and origin of study area. The grid size is selected next. The surface grid sizes commonly used at present are 2×2, 3.2×3.2, and 5×5 km (1.2×1.2, 2×2, and 3.1×3.1 miles). However, the size of each grid will determine the size of the entire study area. At present, the maximum number of grids allowed in regional models varies from 25×25 to 50×100. Therefore, if a grid size of 3.2×3.2 km (2×2 miles) on a side is selected and the model has a maximum of 25×25 grids, then the study area will cover an area of 80×80 square kilometers (50×50 square miles).

In some cases, to expand the grid size requires changes in the computer program. Therefore, care must be taken not to exceed the maximum number of grids. Once the origin and grid size have been selected, then all the emissions for mobile and stationary sources must be located based on this coordinate system and grid. In general, the emission inventory for mobile and stationary sources is developed by different agencies. In California, for example, vehicular emissions are developed by the California Department of Transportation, and stationary emissions are developed by local air pollution control districts or the California Air Resources Board (ARB). Each agency has a different coordinate system to geocode emission sources. This can create problems for the user in acquiring data for each grid square and allocating the proper emissions from both mobile and stationary sources.

Emission Inventory

Emission input into a regional model is generally developed by separate agencies. Problems that arise in obtaining emissions are numerated below.

1. It is difficult to obtain vehicle kilometers traveled allocated to each grid square calculated from transportation models.
2. Transportation simulation models used to predict vehicle kilometers traveled are insensitive to changes in gasoline prices, and that may affect predictions of vehicle kilometers traveled.
3. No recent verification studies have been made of transportation simulation models to evaluate their predictive capabilities based on current travel behavior.
4. In predictions of future vehicle kilometers, the present transportation simulation models cannot respond to changes in highway assignments when gasoline prices are doubled or transit alternatives are considered.
5. Growth rates in present transportation models may not be representative of future trends in population growth within the local community.
6. The ability of transportation models to predict speed on links without some hand adjusting is doubtful.
7. The representativeness of the highway cruise-mode emission factors as published by EPA is questionable.
8. The aircraft emission data are not available as required by air quality models.
9. Stationary source inventories are not up to date and are generally 2 to 3 years behind.
10. Future stationary source inventories from local and state agencies are difficult to obtain.
11. Different air pollution agencies have no consistency in defining reactive hydrocarbons, and this makes it almost impossible to use second-generation kinetic mechanisms that group hydrocarbons into 5 classes of methane, paraffins, olefins, aromatics, and aldehydes.

Existing Meteorological Data Bases

The existing sources of meteorological data for use in regional models are primarily airports and air pollution control district air monitoring stations. The meteorological data monitored consist of surface wind speeds and directions, and in some instances, information from 2 daily radiosonde releases to obtain the vertical temperature profile data. Before examining the existing data, one must keep in mind that the meteorological data will be used to calculate the representative 1-hour wind flow fields on a temporal and spatial basis for the entire study area for each grid. The same applies to the temperature measurements that the existing data must be able to represent and describe the temporal and spatial changes of inversions for the entire area. The following problems arise when existing data are used.

1. In most areas, there are too few ground stations to describe the surface wind flow field.
2. In many cases the instruments to monitor surface winds are insensitive to low speeds less than about 1.35 m/s (3 mph).
3. The readings recorded at airports are generally instantaneous and are not generally representative of the 1-hour average.
4. The air pollution control district wind stations are generally located on tops of buildings and monitor the localized air flow around and over the building and not the representative surface winds.
5. In regions where terrain effects alter the inversion by thermal heating, 1 or 2 radiosonde releases are not representative for the region, nor are they sufficient to describe the temporal behavior.
6. Virtually no measurements are made of winds aloft.
7. Virtually no measurements of insolation are made. If they are, it is generally at only 1 location. This makes it difficult to account for spatial variation in radiation intensity in large urban areas.

Existing Air Quality Data Base

Most of the existing ground air monitoring stations operated by state and local air pollution control districts are located at sites (a) where real estate is inexpensive and (b) where stations are not a great distance apart so that instrumentation technicians can service and check the daily operations. These stations are not located or intended to be used to provide input to a data base or verify regional air quality models. The following problems exist with existing air quality data.

1. The number of ground stations is insufficient to describe the temporal and spatial distribution of pollutants for establishing the initial concentration fields for model inputs or to provide a satisfactory data base to verify models.
2. There are no standards for exposing the air intake or locating the stations. Most stations are located near major surface streets and monitor the local exhaust emissions from vehicles. To confuse the situation further, there is no standard height that the air intake must be above the ground surface. Based on our experiences, the height of the air intake can vary from a 1- to an 8-story building. With this kind of exposure (low air intake and near surface streets), the air monitoring stations generally monitor high concentrations of CO, HC, and NO_x because of nearness of the source. However, reduced values of O_3 may be monitored because of the reaction of NO (emitted from motor vehicles) and ambient O_3 resulting in higher NO_2 concentrations and a depletion of O_3. The reverse may be true when air intake is located on a tall building, i.e., low CO, HC, and NO_x concentration and high O_3. Therefore, the representativeness of these stations is questionable for use as regional modeling input and verification.
3. Air quality measurements aloft are virtually lacking in urban areas. This information is important in determining the initial concentration fields in the models and is also required to treat the O_3 buildup beneath the elevated inversion that can vary from

day to day.

4. Air quality instrumentation used is not comparable from one location to another. Wet chemical methods are used in some urban regions, and dry chemical techniques or a combination of both is used in others. This does not provide continuity in measurements unless careful correlation of instruments is made.

5. A frequent program of calibrating the instruments used in air monitoring stations is lacking. This is necessary to ensure quality data for model applications. Based on our experiences, the frequency of calibration varies from 6 months to 3 years. More typically, it is 1 year or more.

6. The ability of all stations within a network to monitor reactive and total hydrocarbons (RHC and THC) is lacking. In some urban areas only selective stations monitor RHC and THC, and almost all monitor THC. A few partial stations monitor for O_3 only.

Verification of Photochemical Models

Confidence in using regional photochemical models can only be achieved when model predictions are compared to real-world measurements. At present, with the exception of EPA's St. Louis study, not a great deal of attention has been given to monitoring programs to provide measurements of air and meteorological data at the surface and aloft that can be used as inputs to verify regional photochemical models. This should be obvious from the previous discussions. In many instances, reviewing agencies, such as EPA, require that, before a model is used for decision making, the predictions made by the model be compared to actual field measurements and the performance of the model be evaluated accordingly.

Customizing Regional Models for Urban Areas

To our knowledge, all of the existing photochemical models (1, 3, 4) were developed for the Los Angeles basin under contract to EPA. The models developed were, therefore, more of research tools designed specifically for the Los Angeles study area, which is 80×80 square kilometers (50×50 square miles). The computer programs written were customized for the size of the region, the description of the temporal and spatial variation of inversions, and the mountain barriers that alter surface winds for the Los Angeles area. Therefore, to use the existing programs for other regions requires internal changes in the computer code. This is an additional cost to users whether they make the changes themselves or contract with the developers of the models.

Institutional Constraints

Because the models were designed specifically for the Los Angeles area, the models were not written in an efficient manner to be applied to other urban areas. For example, to take the grid model of Systems Applications, Inc. (SAI) and expand the original 25×25 grid system to 50×100 grids (which is required in the South Coast air basin in California) and run a 10-hour simulation on an IBM 370/168 computer system would cost about $2,000 a run. This would require about 16 hours residence time on a typical IBM 370/168 system and would mean, if it were practical, that runs would probably have to be made on weekends only. On a comparative basis, running the original 25×25 grid for 10 hours of simulation on the IBM 370/168 system would cost about $240 with a residence time of about 2 hours in the computer center. On the other hand, studies made by SAI have shown that, if the same programs were converted to a CDC 7600 computer system and run at the Lawrence Berkeley Laboratory, the cost would be reduced by about a seventh or $35 and $300 per 10-hour simulation run for the 25×25 and 50×50 grids respectively. This illustrates that, depending on the number of grids and the user's computing system, it may or may not be possible to use the SAI model on a

practical basis.

If a trajectory model (3) is used for the 25×25 grid and run on the IBM 370/168 system, the cost for a 10-hour simulation run for 1 trajectory is about $20. A comparison of the cost of running a trajectory versus a grid model is misleading because to obtain results similar to the grid model output for a 25×25 grid would require hundreds of trajectory simulation runs. The advantages and disadvantages will be discussed in a later section.

There are some other general operational problems with the existing regional models. The regional models were developed by chemists, physicists, meteorologists, and engineers rather than by transportation planners or highway engineers. Difficulty arises in interfacing the vehicular emission output from transportation simulation models into the air quality model. The emissions depend on the number of links, type of trip, and temporal patterns. The model developers need to coordinate their efforts to provide a more workable package for users. Another problem that arises is that the user instruction manual written by the developers of the air quality models is not oriented for highway engineers but is more suitable for computer programmers. Therefore, the instruction manual needs to be rewritten so that air quality models can be more generally implemented. The computer programs also need to be rewritten to make them more efficient.

SOLUTIONS TO UPDATING AIR QUALITY DATA BASES FOR AIR QUALITY MODELS

The above discussion made it apparent that, in the user's view, the quality of input into regional air quality models has a high degree of uncertainty. In addition, there are computer operational problems. Input includes the emission inventories and the aerometric data bases. High quality of input variables used in the models can result in a more systematic and scientific evaluation of model performance. This conclusion assumes that the user has confidence in the concept of mathematical modeling and confidence in the ability to improve on the model predictions. One part of improving model inputs and predictions requires a field monitoring program to collect an aerometric data base. The design of this aerometric data base should be based on obtaining measurements that are spatial and not point oriented. This means that the location of the measurement points should be based on the model assumptions. In the other part, improvements must be made to obtain a satisfactory emission inventory for mobile and stationary sources.

Before the field program is designed and additional costs are incurred to improve the emission inventories, a sensitivity analysis of the models should be made. The sensitivity can refer to the extent to which the predictions of a model are influenced by a variation in a particular input parameter. Thus, we want to focus on the accuracy of the data used and the sensitivity of the model to variations (or uncertainties) in input data. It is important to determine the magnitude of sensitive parameters as accurately as possible. Little effort should be expended on improving the accuracy of relatively insensitive parameters. Sensitivity analyses (5) made on the SAI airshed model indicate that wind speed, mixing depth, radiation intensity, and emission rates are the most sensitive parameters. A sensitivity analysis of DIFKIN (6) indicated similar results, but also illustrated that the initial concentrations of HC and NO were sensitive parameters. Once we have an indication of what input parameters are most sensitive, it becomes a problem of designing a program to obtain quality inputs with minimal costs.

The following process describes the program followed by the California Department of Transportation to provide the highest quality data for use in regional photochemical models. This department was the lead agency in coordinating and completing the tasks described below.

Study Area

Defining the study area is the first task that must be completed before acquiring a data base. The inputs into regional modeling require the expertise of multidisciplinary groups and agencies. To resolve any conflict in defining the study area requires consultation with local planning agencies, air pollution control districts, state air resources board, EPA regional office, FHWA regional office, National Weather Service, and U.S. Department of Transportation. A multidisciplinary group can ensure that the boundaries of the study region provide for a common base line to include input of meteorology, pollutant emissions, and local land use plans. A group decision eliminates possible challenge as to the appropriateness of the selected region.

Emission Inventory

The next step is to obtain an accurate up-to-date emission inventory for mobile and stationary sources. Because the sensitivity analysis indicates that emission from mobile sources is an important parameter, justification within the California Department of Transportation was given to authorize expenditures to obtain the best state-of-the-art data.

Within the department, a computer program was developed to calculate vehicular emissions by using transportation simulation (7) models and a vehicular emission model (8). Both of the models were interfaced, and emissions were calculated for each link as a function of speed and then aggregated into grid emissions. The emissions were based on trip type, i.e., home to work, home to other, and so on. The emission model was based on the latest data available from EPA and ARB. The emission factors included the latest information on emission standards for light- and heavy-duty vehicles, speed adjustment factors, deterioration factors, vehicle mix distribution, and kilometers traveled per vehicle type for conditions in California. In some cases, the transportation simulation model was recalibrated based on more recent vehicle counts to reflect the changes in travel behavior caused by increased gasoline prices. This effort was felt to be essential in updating the vehicular emission inventory.

The latest update in aircraft emissions was obtained by contacting local airports in regard to the latest schedules of departures and arrivals. The latest aircraft emission factors available from EPA (9) were used to calculate the emissions. In one urban area, the local air pollution control district provided the updated aircraft emission inventory.

To obtain the updated stationary emission inventory, we held several meetings with local air pollution control districts. The results of the sensitivity analysis showed that stationary emissions are a sensitive parameter and that their best estimates for stationary emission would be required to obtain the best results. In most cases, unfortunately, the air pollution control districts provided inventories that were 2 years old until later inventories are updated and completed.

In the development of the emission inventories (mobile and stationary) it is strongly urged that the Universal Transverse Mercator (UTM) system be used to geocode both vehicular and stationary source inventories to ensure that emissions are allocated to the proper grid squares within the study region.

Field Monitoring Program

The next step is to design a field monitoring program to collect an aerometric data base. This data base has a dual purpose: (a) establish an input data base to describe the typical and worst day meteorological conditions and (b) establish a data base to compare predicted concentration with actual measured data. This design made use of all existing sources of data that were located with proper exposure based on the assumptions of the models.

To supplement the existing sources, the department used what instrumentation it had available and designed a new field air monitoring program. In the design of the field

monitoring program, the following persons were consulted: air pollution control district meteorologists, meteorologists of ARB, consultants from the University of California, regional meteorologists of EPA, and meteorologists from the National Weather Service.

This team of experts decided where to locate surface wind stations, pibal release points, radiometers, additional ground air monitoring stations, and aircraft flights to measure temperature and air quality aloft. These instruments were located to best represent the temporal and spatial behavior of meteorology and air quality for the region investigated. The respective agency reduced and provided hourly average data that could be used for model inputs. All information was then coordinated by the transportation department and edited for final input into the models. The field monitoring program was designed to cover the primary and secondary pollutant seasons. For California this corresponds to the months of December through February for the primary pollutants and May through October for the secondary pollutants. Sampling continuously through these months should provide sufficient data to examine model predictions for comparison with observed data over a wide range of meteorological conditions and air quality concentrations. The estimated cost for the Sacramento study (based on California rates) for equipment (wind stations, bag samples), 3 air quality trailers, labor for data acquisition, and data analysis and model verification was $200,000. This cost covered sampling in the Sacramento area (40×40 square kilometers or 25×25 square miles), which is flat and has no local terrain effects and no major point sources. In areas where terrain effects alter surface winds and major point sources exist, such as in San Diego, additional wind stations and air monitoring stations are required and increase the cost considerably. The point that we emphasize is that to collect an aerometric data base for regional air quality modeling for a relatively small urban area requires a major effort in equipment availability and initial expenditures. Unless these data are available, it is not possible to use regional models with any degree of confidence (assuming that the emission inventory is available).

Institutional Constraints

To resolve the institutional constraints as previously described, the transportation department has 2 contracts: one with System Applications, Inc., and the other with General Research Corporation (GRC). The contract with SAI is to provide a working computer program with an expanded grid (50×100) to be run on the CDC 7600 computer. The contract also requires that a user documentation manual be prepared and that formalized training for department personnel be provided. Similarly, the contract awarded to GRC is to convert the DIFKIN model to the IBM 370/168 computer system with the expanded grid and to provide a training course. The total price of both contracts required an initial investment of approximately $100,000.

IMPLEMENTATION OF URBAN AIR QUALITY MODELS

The transportation planners and engineers have 2 types of air quality models from which to choose: grid model and trajectory model. As previously mentioned, in the grid model the airshed or study region is divided into a 3-dimensional grid, each cell being perhaps 2 km (1.2 miles) on a side and a few hundred meters high. The grid is then used as a basis for the numerical integration of the conservation-of-mass equation. In the trajectory approach, a hypothetical column of air is followed through the region as it is advected by the wind. Pollutants are emitted into the column, and chemical reactions take place within the column. Based on our experiences, both modeling approaches have the following advantages and limitations depending on the application.

Advantages of a Trajectory Model

1. The model is applicable for project level analysis. Figure 2 shows this application for a given highway project. For this application, the proposed highway was divided into 3 equal segments. The air parcel began over the ocean and eventually reached the segment 1 at 7 a.m. The path of the trajectory is indicated by path ABCDEFG. The actual path of the trajectory continues along the path H... P. The grid size is 3.2×3.2 square kilometers (2×2 square miles). Pollutant concentrations are predicted along the trajectory only.
2. The model can locate sources that produce hot spots for pollutant emissions.
3. Pollutant concentrations can be predicted in valleys because of the ability of the trajectory model to simulate air movements in valleys by using an air parcel approach.
4. The model is applicable to areas where terrain affects surface winds.
5. For a given trajectory, the model is computationally efficient and can be run on most computers at a reasonable cost.

Limitation of a Trajectory Model

1. The model is not directly applicable for convergent or divergent wind flow fields.
2. The model is not applicable where vertical wind shear is an important consideration.
3. The model is not applicable for transportation systems planning because of the numerous trajectories required to locate hot spots or areas where high concentrations occur.
4. The trajectories calculated are sensitive to the exposure of wind stations; therefore, surface wind data used as input must be consistent with model assumptions.
5. It is difficult to directly compare the trajectory model prediction of air concentrations at a given location or grid with the hourly National Ambient Air Quality Standards.
6. Large volumes of input data are required.

Advantages of a Grid Model

1. The model is applicable for system planning to determine the interrelations of land use, transportation, and air quality. Figure 3 shows the typical output for spatial concentrations of O_3 in pphm for the Los Angeles area.
2. The model is applicable to areas where terrain effects alter surface winds.
3. The model is applicable to areas where a convergent or divergent wind flow field exists.
4. The model is applicable for areas where wind shear is important.

Limitations of a Grid Model

1. It is expensive to run simulations on most computer facilities.
2. The model is not applicable to project-level analysis because of the expense in running the model.
3. The numerical solution of the partial differential equations introduces artificial diffusion problems and inaccuracies in the output if model runs simulate more than 10 hours.
4. Large volumes of input data are required.

Conclusions

Clearly, transportation planners and engineers must decide on the type of problem they

Figure 3. Typical output from SAI airshed model for Los Angeles.

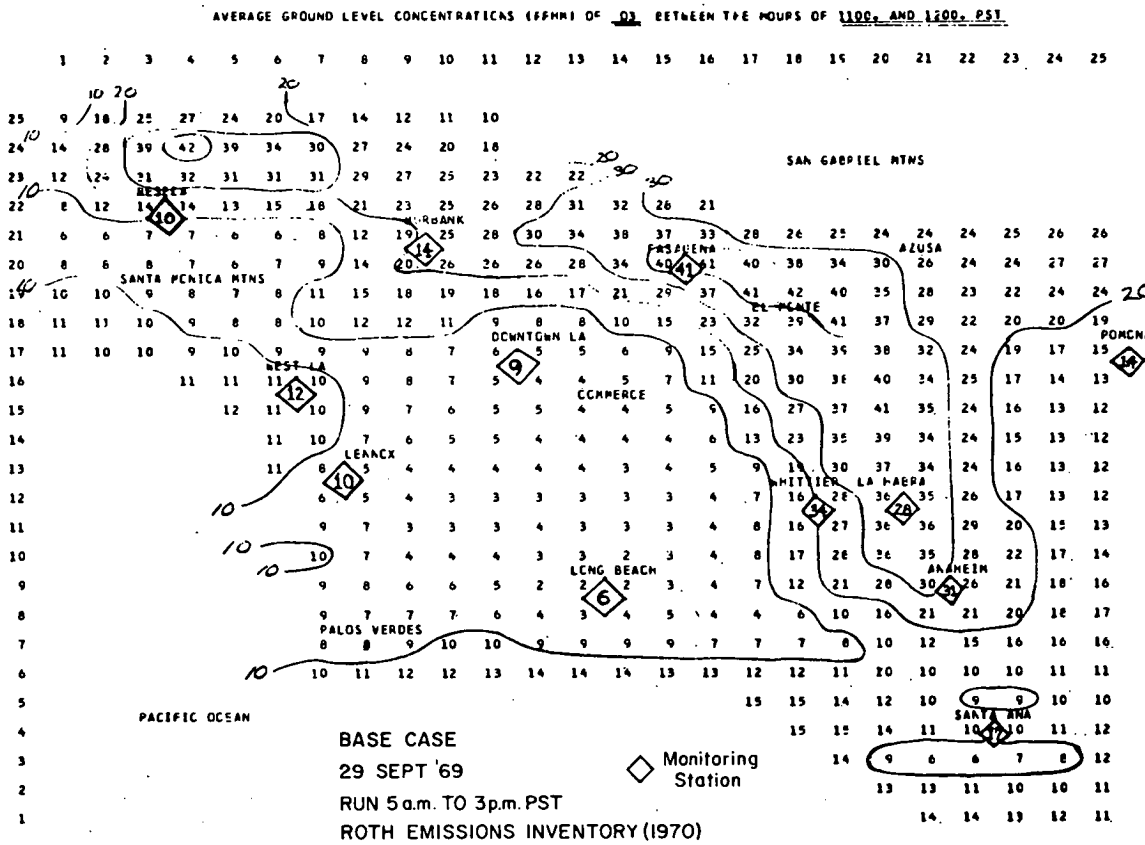
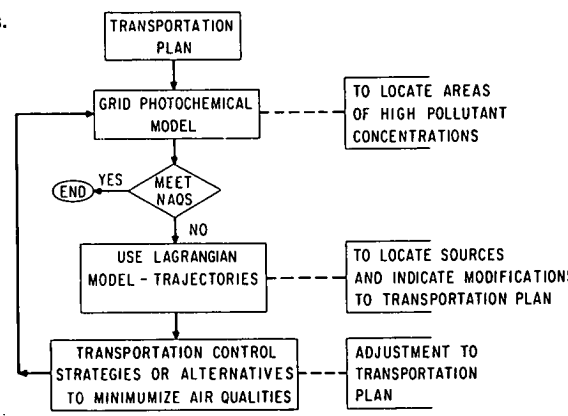


Figure 4. Flow chart for systems analysis.



want to evaluate and consider the possible trade-offs in modeling approaches. The user must select the model that is most cost effective for the desired application. The California Department of Transportation at present feels that both modeling approaches should be integrated in their application for transportation planning. First, the grid model is applied to evaluate the air quality of a proposed transportation plan. Using a grid model enables one to locate areas of high pollutant concentrations. Once the hot spots are located for a certain meteorological condition, a backward trajectory is then made by using a trajectory model to locate the respective emission sources in grids that cause the high concentrations. Next, a modification for the transportation plan is made to reduce the areas or grids of high pollutant emissions by perhaps considering spatial, temporal, or modal alternatives. Finally, the grid model is rerun to see whether the modifications to the transportation plan have reduced the hot spots and have not necessarily affected or altered the air quality in other areas. This process is repeated until a trade-off is reached. Figure 4 shows the use of the grid and trajectory photochemical models for systems planning.

Both modeling approaches have the common problem of requiring a large input data base, which initially is expensive to develop. Even with this initial investment to operate trajectory or grid models, transportation planners and engineers should consider the other alternative modeling approach available to them: rollback. A careful examination of whether rollback can evaluate spatial alternatives of emissions and their effect on quality will clearly indicate it cannot. Regional photochemical modeling is, at present, the only approach to provide rational answers to the complexity of today's problems. Confidence in any model can be achieved only by comparing predicted concentrations with observed data.

SUMMARY

This report discusses from the user's point of view the applications of regional photochemical models to assess the interrelations of land use, transportation, and air quality planning. It discusses the problems with using existing emission and aerometric data and presents solutions to remedy these problems. Institutional constraints to running computer simulation models on various computer systems are discussed. The advantages and limitations of trajectory and grid models are discussed for transportation systems analyses.

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Discussion

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It is appropriate that Ranzieri and Shirely discuss at length problems of data acquisition for providing input to models. In this discussion, the counterpoint of solutions to these problems will be emphasized. Although these comments are from a developer's as well as a user's point of view, it should be noted that it is not my intention to endorse in a wholesale fashion or defend for all purposes the application of regional photochemical models.

Computer simulations, graphs, and formulas that may be called air quality models provide a vast array of possibilities on different levels from which to attack the problem of forecasting long-range trends in air quality as a function of emissions. Mathematical formulations that relate long-term averages to short-term averages or that relate air quality to meteorological variables are models of a sort; however, the term "air quality models" as defined here will be those means of evaluating emission control strategies.

DATA BASE

From a philosophical point of view the quality of the data base and the quality of the model formulation must not be confused. It is an oversimplification to say that a model does not perform well because of unknown uncertainties in the input data. Likewise, more precise statements than those made previously regarding the meaning of sensitivity can be formulated. For example, if it is found that the buildup of photochemical oxidant is extremely sensitive to the choices of nitric oxide flux at the ground, then we have encountered a manifestation of the extremely fast reaction of nitric oxide with ozone. In this example, it is incorrect to say that something is amiss with the model formulation because of a high degree of sensitivity. A more useful interpretation of this finding is that we must know the emission data base with relatively good accuracy for nitric oxide emissions if we are to predict oxidant buildup with any degree of confidence by using any model that captures the true chemistry.

The concern about nonstandard grids that is expressed by the authors is a real one in practical studies. Invariably the planning agencies, their consultants, the transportation agencies, and the environmental control agencies have slightly different views toward methods of data storage. A continued push is being made toward the application of Universal Transverse Mercator grid systems for the wide variety of emission-related data needed for inputs in photochemical diffusion models.

Probably the single most significant input feature for these models is an accurate space and time distribution for emissions of all primary pollutants. Standard data bases now have these emissions by county and not by grids as implied by Ranzieri and Shirely. We have found that these aggregated statistics may be geographically distributed according to land use maps with grid overlays. The output accuracy of transportation network

flow simulations is really a problem separate from air quality modeling; however, it is one that must be considered by transportation planners for a variety of purposes including environmental quality predictions. As indicated later by the authors, computer packages are available for distributing the vehicle movement statistics from transportation simulations to rectangular or square grids used for air quality modeling. This is another area where the authors place more emphasis on the problems than on the solutions.

Although valid application of air quality models depends on truly representative meteorological and air quality data, there are very few cases where this will be available. The authors leave the reader with the dilemma that none of the data is good enough to use in existing models and that the alternative of rollback estimates is also unacceptable. Two messages should emerge from this dilemma: (a) Agencies that collect the data should be encouraged to exercise greater care in siting and measurement, and (b) models that can tolerate corrupted data should be developed for the near term.

In cataloging the data base problems, the authors give only slight emphasis to one of the largest outstanding problems for the modeling of photochemical oxidant regardless of what type of coordinate frame is used for a photochemical diffusion model. That problem is the detailed hydrocarbon inventory needed by the so-called second-generation photochemical diffusion models. At the present time it is difficult enough to obtain geographical and time distributions of reactive hydrocarbon emissions. The newer model versions, however, require an allocation of the reactive hydrocarbon emission into chemical classes such as paraffins, olefins, aromatics, and oxygenates. No control agency maintains files of such finely broken down hydrocarbon inventories. Nevertheless, there is a way out of this problem too. That is to consult some of the recent literature on reactivity assessments that gives rather detailed compound class breakdown to emissions from different types of pollutant sources. These approximate distributions can be folded in with aggregate reactive hydrocarbon inventories to obtain the needed distributions for future modeling.

APPLICATION OF EXISTING MODELS

The authors make repeated reference to comparison of model predictions with "real-world measurements." The existence of recently completed and ongoing field-measurement programs seems to be totally overlooked. Many millions of dollars have been spent by the California Air Resources Board in surveying 3-dimensional pollutant gradients, in tracing the movement of air masses in California air basins, and in measuring the composition as well as rate of appearance of photochemical aerosols. The Coordinating Research Council in conjunction with the National Oceanic and Atmospheric Administration and with the U.S. Environmental Protection Agency has completed the Los Angeles Reactive Pollutant Program, which provides an extensive data base designed for the verification of models. For the past several years and at the present, EPA is conducting the Regional Air Pollution Study in St. Louis expressly designed for the purpose of providing a validation data base for regional air quality models. In view of these efforts, it cannot be said, therefore, that "there has not been a great deal of attention given to measurement programs to provide input to verify regional photochemical models."

This comment is not intended to say that all the problems are solved, because in many cases measurement programs designed for model validation have not followed the statistical rules of experimental design, but rather have been constrained by logistical necessities. This means that future evaluation studies of models will still be hampered by data sample limitations; however, the scope of the measurements in the present round of field programs is so great that testing will now be possible for portions of models that have gone unchecked until now.

The outcome of these verification tests for different regions must be a set of performance parameters that can be applied to any model. The user can select the model on the basis of how well certain performance parameters are met. Naturally it is not the optimal solution to use the model with the highest degree of accuracy for all applica-

tions. Many cases of evaluation of future alternative decisions require a rank ordering or comparison rather than a specific calculation of a concentration level. Other cases require the probability of exceeding a certain threshold pollutant level rather than the complete computation of an ensemble of conditions.

It is difficult to compare costs in operation of models unless it is done in a rather gross sense. When actual dollar values are quoted, they must be carefully qualified by answering the question "costs to whom?" How many control agencies or transportation planning groups have access to CDC 7600 or STARR computer systems? The appeal for rewriting computer programs to increase efficiency is a good one and should be implemented by using recently developed numerical integration algorithms. In the category of other issues to be resolved before using regional photochemical models, there is now a substantial collection of aerometric data bases against which model assumptions can be tested. Again it should be emphasized that the fidelity of a model is not measured by its sensitivity to input data. In the example given previously, high degrees of sensitivity actually indicated a physical or chemical reality rather than a flaw in the mathematical formulation of the model. Commenting specifically on the sensitivity parameters discussed in the paper, it should be noted that grid models such as those developed by SAI and by Environmental Research and Technology, Inc. (ERT), depend on accuracy of initial conditions and edge conditions in addition to wind speed, mixing depth, and other parameters indicated in the paper. Lagrangian models such as DIFKIN exhibit this sensitivity in the assignment of initial concentrations. Because of the interchange of time for space, the need for accuracy in edge conditions translates into a need for accuracy in initial conditions.

Some of the limitations in both trajectory and grid models can be circumvented by careful applications and modifications. For example, vertical velocity modifications in the trajectory model will render it applicable for convergent or divergent flow fields. Shear corrections currently incorporated permit an accounting for this physical effect. The use of trajectory models for systems planning will be possible by using the multi-trajectory grid version of atmosphere reaction and transport simulation (ARTSIM) now under development at ERT. It is true that both types of models are sensitive to the exposure of wind stations and that surface wind data used as input must be consistent with model assumptions.

Regarding limitations on grid models for project level analysis, a limited portion of the grid may be treated for project level analysis at much lower expenditure of computer costs. The numerical problem of artificial diffusion has been overcome by the Egan and Mahoney code using conservation of moments that allows subgrid scale elements of contaminant to be treated in the advective portion of the program. Finally, both types of approach will benefit from more rapid numerical integration techniques that are being introduced by several groups.

IMPROVEMENTS IN THE MODELING ART

As mentioned in the previous sections, a number of features have been introduced to upgrade existing models. Even after this occurs, however, we are still faced with the dilemma of using either a relatively complicated physical-chemical formulation to predict oxidant levels or an inadequate data correlation called rollback. Up to now there are few available intermediate solutions that relate emissions to air quality (recall the cautions in the introduction regarding statistical models relating air quality to nonemission variables).

What is needed then is the invention of a new model that can be operated with existing data that may be insufficient for the photochemical diffusion models. The objective of such a model would be to relate emissions to air quality in only the degree of refinement required for evaluating emission control strategies. Very specifically this translates into a requirement to predict the number of violations of the National Ambient Air Quality Standards (NAAQS) and not the case-by-case or hour-by-hour prediction of concentrations at every point in an airshed. Another objective is that the model content be expressible in a simple enough algorithm that control agencies and transportation planners

who possess little specialist training in meteorology and chemistry can use the models.

An approach to this problem can be found in the use of cluster analysis. In this form of analysis a dependent variable is classified into clusters as determined by values of an independent variable. For example, we might take individual hours that violate the NAAQS and designate them with a V for violation, then take those hours that do not violate the NAAQS and designate them by an N for nonviolation. The next step might be to plot Vs and Ns with a graph of mean daily temperature versus emissions into an air parcel arriving at each particular hour. If this is a good choice of independent variables, we will have 2 clusters of Ns and Vs that show little overlap. This degree of knowledge is important for designing control strategies because it tells us what causes are in operation to bring about violations or nonviolations. This is one example of a type of model that may be developed to supplement rollback or diffusion modeling.

CONCLUDING REMARKS

Although data base problems exist, they are not insurmountable. Uniformity has been attained in many cases where commonality in land use, traffic, and resource inventories is achieved. Meteorological and air quality data bases are growing, and the awareness of correct sampling or calibration procedure is developing in many agencies. Although existing models may be adapted to special cases of either transportation project studies or system studies, their degree of complexity will be growing as physical and chemical improvements are introduced. The so-called second-generation models require levels of input data far beyond those that will normally be available. Therefore, they must be looked on as testbeds for concepts in air pollution control and for interpolating or projecting details in air quality distribution such as "hot spots" with respect to sources or receptors. General control strategies will probably use cruder models than these highly refined finite difference computer simulations. The crudeness will not extend to the level of simple rollback, but rather will include the basic chemical and meteorological factors influencing air quality in the future. We wholeheartedly agree that the rollback procedure cannot provide answers to problems of predicting concentration in the future. These strategies will involve, in some cases, unusually severe economic and social dislocations; therefore, we will strive for timely and reliable predictions using information that is typically available from existing data sources.