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Application of Photochemical Models

Volume IV

A Comparison of the SAI Airshed Model and the LIRAQ Model

APPLICATION OF PHOTOCHEMICAL MODELS

Volume IV

A Comparison of the SAI Airshed Model and the LIRAQ Model

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PREFACE

This document is one of four volumes intended to provide information relevant to the application of photochemical models in the development of State Implementation Plans. The reports are particularly directed toward agencies and individuals responsible for preparation of non-attainment plans and SIP revisions for ozone. The four volumes are titled as follows:

Application of Photochemical Models

Volume I - The Use of Photochemical Models in Urban Ozone Studies

Volume II - Applicability of Selected Models for Addressing Ozone Control Strategy Issues

Volume III - Recent Sensitivity Tests and Other Applications of the LIRAQ Model

Volume IV - A Comparison of the SAI Airshed Model and the LIRAQ Model

This work is to a large extent based on the photochemical modeling experience gained in the San Francisco Bay Area in support of the 1979 Bay Area Air Quality Plan. The following individuals made significant contributions to this work:

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A COMPARISON OF THE SAI AIRSHED MODEL AND THE LIRAQ MODEL

Federal legislation requiring the preparation of various environmental assessments--such as State Implementation Plans [SIP(s)] and New Source Reviews [NSR(s)]--has motivated the development of several types of air quality models. The primary purpose of these models is to provide a quantitative relationship between source emissions and the resulting ambient air quality levels. Formulation of a suitable model for photochemical oxidants is particularly difficult since complicated chemical transformations are responsible for the process by which emissions of reactive organic compounds and nitrogen oxides (mainly NO) lead to the formation of ozone, NO_2, peroxyacetylnitrate, and various other oxidants. Several models have been published in the technical literature ranging from the relatively simple linear and modified rollback schemes to the more sophisticated trajectory and grid models.

At the present time, the Environmental Protection Agency (EPA) is faced with the need to provide guidance to the various local and state agencies responsible for preparing revisions to State Implementation Plans with regard to the modeling procedures to be employed in carrying out photochemical oxidant analyses. Over the past several years, considerable effort has been devoted to the development of two sophisticated grid-based photochemical air quality simulation models. Since 1970, the Systems Applications, Incorporated (SAI) Airshed Model has been the subject of continued developmental work funded largely by the EPA and U.S. Department of Transportation. The Livermore Regional Air Quality (LIRAQ) model has similarly evolved from a multiyear research and development effort conducted by the Lawrence Livermore Laboratory (LLL) and funded by the Research Applied to National Needs (RANN) section of the National Science Foundation. We note that these models are representative of the state of the art in photochemical air quality simulation modeling at the present time.

The purpose of this report is to compare the various technical features of the SAI Airshed Model and the LIRAQ model. Since detailed mathematical descriptions of each model have been published in various technical journals and reports, we confine our presentation here to a general description of the similarities and differences of each model. We envision that this report will fill three needs. First, it should give the participants in this study a good overall description of the two models, which will be helpful in the development of the guidance documents to be prepared in this contract effort. Second, it should prove useful to potential model users who may be trying to decide which of the two models to employ in some air quality assessment study. A good understanding of each model is essential to sound decision-making regarding model selection. And third, this document should help EPA personnel in their ongoing photochemical model applications studies, especially those that involve direct comparisons of these two models.

We note that this report is being prepared to aid the EPA Office of Air Quality Planning and Standards (OAQPS) in its attempt to obtain a better understanding of the relative strengths and shortcomings of these two rather complex photochemical models. To this end, OAQPS personnel are going to adapt the SAI Airshed Model for usage in the San Francisco Bay Area. Once this is done, the two models will be exercised using inputs derived from the same data base. Analysis of the results generated by each model should provide some insight into their relative performance. In a companion report written by Reid and Reynolds (1979), guidelines are given for constructing inputs for the SAI model using the information contained on the available LIRAQ input files.

In structuring our presentation in this report, we begin in Section A by examining the governing equations of each model. In Section B, the discussion focuses on the various treatments of atmospheric processes, such as emissions, transport, chemical reactions, and removal. Section C is devoted to a comparison of model inputs. We conclude this report in Section D by considering the output produced by the two models.

A. FORMULATION OF THE MODELS

The basis of both the LIRAQ model and the SAI Airshed Model is the continuity equation, which expresses the conservation of mass of each pollutant in a turbulent fluid in which chemical reactions occur. This equation can be written in the following manner:

$$\underbrace{\frac{\partial c_i}{\partial t}}_{\text{Time Dependence}} + \underbrace{\frac{\partial (uc_i)}{\partial x} + \frac{\partial (vc_i)}{\partial y} + \frac{\partial (wc_i)}{\partial z}}_{\text{Advection}} = \underbrace{\frac{\partial}{\partial x}\left(K_H \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V \frac{\partial c_i}{\partial z}\right)}_{\text{Turbulent Diffusion}}$$

$$+ \underbrace{R_i}_{\text{Chemical Reaction}} + \underbrace{S_i}_{\text{Emissions}} , \qquad (1)$$

where c_i represents the pollutant concentration and is a function of space (x,y,z) and time (t). This equation describing the dynamic behavior of reactive pollutants is fully three-dimensional and is used directly in the SAI Airshed Model. To obtain the governing equation of the LIRAQ model, additional assumptions are invoked to derive a suitable two-dimensional form of Eq. (1).

Examination of Eq. (1) indicates that the following physical and chemical processes are considered in the Airshed Model:

- Pollutant advection. The model can treat a fully three-dimensional wind field, where u, v, and w are the mean wind velocity components in the x-, y-, and z-directions, respectively.
- Turbulent diffusion. Pollutant transport resulting from the influence of atmospheric turbulence is treated through the use of the eddy diffusivity concept; K_H and K_V are the horizontal and vertical diffusivity coefficients, respectively.

- Chemical reaction. The term R_i represents the net rate at which pollutant i is generated by chemical reactions. The reaction rate is a function of pollutant concentration, temperature, and the intensity of ultraviolet radiation.
- Emissions. The spatial and temporal distribution of the source emissions are treated in the term S_i. For large point sources, the total effective plume rise is calculated to enable the appropriate spatial placement of the emissions aloft.

In addition, removal of pollutants by surface uptake processes is considered in the boundary conditions of Eq. (1).

To derive Eq. (1) from the fundamental continuity equation three assumptions are necessary: first, pollutant transport effects due to molecular diffusion are small relative to those attributable to turbulent diffusion; second, pollutant transport due to turbulence can be adequately parameterized through the use of the eddy diffusivity concept; and third, turbulent concentration fluctuations have a negligible influence on reaction rates. For a more thorough discussion of the derivation of Eq. (1), we refer the reader to the reports by Reynolds et al. (1973) and Reynolds, Seinfeld, and Roth (1973).

Because the set of equations is both nonlinear and coupled (through the reaction terms R_i), Eq. (1) cannot be solved analytically; therefore, appropriate numerical techniques must be utilized to find an approximate solution. To facilitate the application of finite difference methods in the SAI model, the vertical dimension is normalized to the distance between the bottom and top of the modeling region. This step is accomplished by defining a new independent variable ρ:

$$\rho = \frac{z - H_b(x,y,t)}{H_t(x,y,t) - H_b(x,y,t)}$$

where H_b and H_t are the elevations of the bottom and top of the region, respectively. Upon performing this change of variable and neglecting cross-derivative turbulent diffusion terms, Eq. (1) becomes (Reynolds, Seinfeld, and Roth, 1973):

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial x}(u\Delta H c_i) + \frac{\partial}{\partial y}(v\Delta H c_i) + \frac{\partial}{\partial \rho}(W c_i) = \frac{\partial}{\partial x}\left(K_H \Delta H \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \Delta H \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial \rho}\left(\frac{K_V}{\Delta H}\frac{\partial c_i}{\partial \rho}\right) + R_i \Delta H + S_i \Delta H \tag{2}$$

where

$$W = w - u\left(\frac{\partial H_b}{\partial x} + \rho\frac{\partial \Delta H}{\partial x}\right) - v\left(\frac{\partial H_b}{\partial y} + \rho\frac{\partial \Delta H}{\partial y}\right) - \rho\frac{\partial \Delta H}{\partial t}$$

and

$$\Delta H = H_t(x,y,t) - H_b(x,y,t)$$

Basically, Eq. (2) with appropriate initial and boundary conditions is the equation whose solution yields the predictions obtained from the SAI Airshed Model.

The Airshed Model provides for segmenting the column of air above each grid square into several cells. These cells may include all or part of the mixed layer or can extend, if one exists, into an elevated inversion layer. If, for example, calculations are performed in the mixed layer only, then, the modeling region would be subdivided into several equally spaced cells in the vertical direction bounded by the terrain and the base of the inversion. To facilitate the calculation of pollutant concentrations within the inversion, a second set of equally spaced cells can be added to the

modeling region bounded, for example, by the base and top of the inversion layer. When performing multiday simulations, these provisions for treating the inversion layer may be important in properly accounting for the effect of pollutant entrainment into the mixed layer as it deepens during the day.

To derive the governing equations for the LIRAQ model, it is first assumed that the wind velocity components can be written in the following manner:

$$u(x,y,z,t) = u_m(x,y,t)\left(\frac{z}{z_m}\right)^n \quad , \tag{3}$$

$$v(x,y,z,t) = v_m(x,y,t)\left(\frac{z}{z_m}\right)^n \quad , \tag{4}$$

where u_m and v_m are the velocity components at height z_m. According to MacCracken et al. (1978), n is normally set to a value of 1/7 to represent neutral stability conditions in the mixed layer. Any other value (except -1) may also be chosen. By invoking further assumptions regarding the transport and chemical reaction processes, MacCracken et al. argue that the concentration profile at any point can be represented by the expression:

$$c_i(x,y,z,t) = a_i(x,y,t) + b_i(x,y,t)\ln\left(\frac{z}{z_0}\right) \quad , \tag{5}$$

where a_i and b_i are parameters that are a function of the mixing depth, source strength, deposition velocity, and eddy diffusivity at a height z_0 (taken to be 1 meter) above the ground, below which the concentration is assumed uniform with height.

Substituting Eqs. (3) through (5) into Eq. (1) and performing a vertical integration from z_0 to the base of an elevated inversion layer yields the following governing equation for the LIRAQ model:

$$\frac{\partial \Delta H' \bar{c}_i}{\partial t} + \frac{\partial}{\partial x}\left[u \Delta H' \bar{c}_i (1+\beta_i)\right] + \frac{\partial}{\partial y}\left[v \Delta H' \bar{c}_i (1+\beta_i)\right] + W_i$$

$$= \frac{\partial}{\partial x}\left(K_H \frac{\partial \Delta H' \bar{c}_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial \Delta H' \bar{c}_i}{\partial y}\right) + \bar{S}_i \Delta H' + \bar{R}_i \Delta H' \qquad (6)$$

where $\bar{c}_i$ is the vertically averaged concentration of pollutant i, $\Delta H'$ is the mixing depth, and $\beta_i = (n/n+1)(b_i \sqrt{c_i})$. The term W_i represents the net effective flux of pollutant i transported through the top of the modeling region:

$$W_i = \begin{cases} W_H \bar{c}_i(x,y,H,t) \ , & W_H > 0 \\ 0 \ , & W_H = 0 \\ W_H c_{T,i} \ , & W_H < 0 \end{cases} ,$$

where W_H is the velocity at the top of the region H, and $c_{T,i}$ is the assumed boundary concentration at H. $\bar{S}_i$ and $\bar{R}_i$ are the vertically averaged values of the source and reaction terms given in Eq. (1). For further details regarding the formulation of the LIRAQ model, we refer the reader to the paper by MacCracken et al. (1978).

In the description presented by MacCracken et al. it is mentioned that the parameter β_i in Eq. (6) was set to zero in the San Francisco applications. Thus, comparing the governing equations for both models [Eqs. (2) and (6)], we note that they are very similar. However, the concentrations predicted by the LIRAQ model are vertically averaged values, though application of Eq. (5) does enable one to obtain an estimate of the ground-level values. In using Eq. (5), if the source flux is larger than deposition, then the near ground-level concentration will be higher than the vertical average concentration, and vice versa. The smaller the value of the turbulent diffusivity, the larger the difference between the ground-level and vertical average concentration. Although the concentration profiles predicted by Eq. (5) are in general agreement with observations, the adequacy of this procedure as a means for calculating ground-level concentration values, especially for ozone, has not been fully evaluated.

No a priori assumptions are made concerning the vertical profile of the winds or pollutant concentrations for the SAI model. The vertical resolution depends on the number of vertical levels used (the current limit is 10 levels) and on how many of those levels lie above the inversion base. The ground-level concentration is taken as the concentration in the lowest layer of cells. An option included in the SAI model (discussed later) adjusts the concentrations in the lowest layer of cells to account for the nonuniform distribution of sources.

Because the LIRAQ and SAI models have evolved from multiyear research and development programs, the available technical documentation is rather voluminous. Therefore, we suggest that anyone desiring additional information regarding the LIRAQ model and its initial application to San Francisco begin by examining the summary papers written by MacCracken et al. (1978), Dickerson (1978), and Duewer, MacCracken, and Walton (1978). More detailed descriptions of the model and a recent application to St. Louis are given in the reports by MacCracken and Sauter (1975), MacCracken (1975), and Duewer et al. (1978). The papers by Reynolds, Seinfeld, and Roth (1973), Roth et al. (1974), and Reynolds et al. (1974) describe early developmental work on the SAI model and its initial application to Los Angeles. The recent report by Reynolds et al. (1979) provides a summary description of the technical features currently embodied in the SAI model and the results of recent applications to Los Angeles, Sacramento, and Denver. A number of other studies carried out by SAI using the Airshed Model are described in the report by Reynolds, Tesche, and Reid (1979).

B. COMPONENTS OF THE MODELS

This section examines the ways in which atmospheric processes are treated in the SAI Airshed Model and the LIRAQ model.

1. Horizontal Transport

Both models treat the two processes that transport pollutants in the horizontal direction--advection and turbulent diffusion. Specification and use of

the horizontal wind is straightforward. For the LIRAQ model, the mass flow at each face of a grid cell is input. Use of mass flow rather than wind speed takes into account any changes in the mixing depth from one edge of a cell to the other. For the SAI model, the x- and y-components of the wind vector are specified at the center of each grid cell. Since there can be more than one level of cells, wind shear (including both speed and direction changes with height) can be accounted for in the SAI model. Although this feature allows the user to represent more realistically the actual three-dimensional wind field, routine meteorological data collection efforts are frequently inadequate for characterizing spatial and temporal variations in the winds aloft. In previous SAI model applications, estimates of upper level wind flows have been generated through the use of available wind soundings and various diagnostic wind models (see Tesche and Burton, 1978; Reynolds et al., 1979; Killus et al., 1977). In general, it is desirable to mount a special field program to measure winds aloft several times during the day in the urban area of interest. This program is important for both models since horizontal pollutant transport is influenced by the winds throughout the mixed layer, not just the winds near the surface (where routine wind data are usually measured).

Though generally less important than horizontal advection, both models also consider horizontal transport by turbulent eddies. To approximate the subgrid-scale transport due to turbulence, it is assumed that the pollutant flux is proportional to the concentration gradient. The proportionality factor is called the eddy diffusivity coefficient. In both models, the horizontal diffusivity coefficients for turbulent transport in the x- and y-directions are equal [as designated by K_H in Eqs. (2) and (6)]. For the LIRAQ model, the values of the horizontal diffusivity coefficients are calculated outside the model by MASCON (described in a later section) using the principles of similarity theory. Basically, the diffusivity coefficient is a function of the wind speed and the mixing depth.

The SAI model uses a constant value for the horizontal diffusivity (50 m^2/sec). Although the horizontal diffusivity treatment in the LIRAQ model is more realistic, the effect on the predicted pollutant concentrations of

using a constant coefficient should be small; studies reported by Liu, Whitney, and Roth (1975) indicated that the model results are not very sensitive to the value of this parameter. This effect occurs because gradients in the concentration field are often relatively small since emissions from point and line sources are spatially averaged over relatively large grid cells. In addition many of the important horizontal atmospheric motions can be represented explicitly in the advection terms of the governing equation through the use of a relatively fine grid covering the urban area. The effects of the remaining subgrid scale motions, which must be parameterized in the diffusivity coefficient, are correspondingly somewhat less important.

2. Vertical Transport

Exchange of material between vertical cells is characterized only in the SAI model, though both models consider exchange of material across the top of the modeling region. As is the case for horizontal transport, there are two components of vertical transport--advection (caused by the vertical wind component) and vertical turbulent diffusion. In addition, the height of the cells can change, thereby causing a flux across the cell interfaces. This term is similar to that generated by the vertical wind component; in both models, these terms are combined to yield a net pollutant velocity relative to each grid cell interface.

The LIRAQ model considers vertical transport at the top of each cell. It is assumed for this model that the effect of material exchange between the mixed layer and the inversion layer as a result of a turbulent transport can be combined into a net advective flux term. This flux at the top of the modeling region is represented by a term that includes any vertical mass flow needed to balance the horizontal mass flows, induced turbulent ablation of the inversion that leads to changes in the cell height due to a raising or lowering of the inversion base in time, and horizontal transport through a spatial gradient in the height of the inversion base. If pollutants are transported or entrained into the inversion layer (and thus out of the modeling region), they are excluded from all subsequent calculations

in the LIRAQ model. As a result, they cannot be reentrained at a later time in the simulation if, for example, the inversion base rises as a result of surface heating effects. The concentration of pollutants in the air entrained into the mixing layer is specified, in part, as a model input. The concentration of pollutants in the inversion is calculated by an empirical function involving the predicted concentration just below the base of the inversion and a user-specified concentration value and scaling parameter (between 0 and 1).

The SAI model has the capability of modeling both the mixed layer and part or all of the inversion layer with one or more levels of cells within each layer. The rate of turbulent diffusion, especially between levels within the mixed layer, must be considered. Again, the assumption is made that the effect of turbulent diffusion is proportional to the concentration gradient in the vertical direction with the proportionality factor, K_V, being the vertical diffusivity coefficient. The SAI model calculates this coefficient for each grid cell interface on the basis of the wind speed, surface roughness, height of the inversion base, height of the cell interface, and the stability class. The stability class within the mixed layer is estimated from the wind speed and solar insolation* (exposure class), and above the mixed layer, it is estimated from the temperature gradient*. Different algorithms for K_V are used for the three possible stability classes: stable, neutral, and unstable. For unstable conditions mixing is rapid, and as a consequence, the vertical concentration gradients are small. Stable conditions produce almost no mixing due to turbulence, and neutral conditions result in modest, but not insignificant, mixing.

The stability in the upper layer of grid cells can be either neutral or stable, thus allowing the treatment of a surface-based inversion capped by a layer of neutrally stable air or a mixed layer capped by a stable layer. For

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* At the present time these variables are assumed to vary temporally but not spatially in the SAI model.

grid cells within an elevated inversion layer, the values of the diffusivities are relatively small, effectively eliminating vertical transport by turbulent diffusion. At the top of the modeling region, the vertical concentration gradient is set to zero if the advective velocity of pollutants relative to the top of the region is equal to zero or is directed out of the region. Otherwise, if material is advected into the modeling region, then the pollutant flux is calculated by multiplying the net velocity times the boundary concentration just above the top of the region.

As in the LIRAQ model, the flow of pollutants relative to a cell interface is made up of three components. The SAI model differs only in the respect that, for every cell except those adjacent to the ground, there is a mass flow through the bottom, as well as the top, of the cell. The mass flow at the top of a cell is calculated using a mass balance that considers the net amount of air carried into the cell by the horizontal wind components, the amount of air injected through the bottom of the cell (from a previous mass balance calculation for the cell below), and any change in height of the cell as a function of time.

The vertical resolution of the SAI model enables it to handle the entrainment into the mixed layer of pollutants that enter the inversion either from elevated point source emissions or at the time the stable layer formed during the previous night. In light of the limited treatment of the inversion layer in the LIRAQ model, the SAI model would be better suited for applications in which large elevated point sources are important or multiple-day simulations are to be performed.

3. Emissions

Emissions of pollutants are divided into two classes, those emanating from either ground-level or elevated point sources. Emissions from mobile sources, distributed area sources (such as space heating, gasoline marketing, solvent usage, and so on), and other stationary sources that do not emit pollutants from tall stacks are generally considered to be in the ground-level

source category. The distinction between stationary sources treated as ground-level sources and those treated as individual point sources is not always clear-cut. The LIRAQ model application to San Francisco designated elevated point sources as those with emissions higher than 30.5 meters. The SAI model applications used a corresponding height of about 50 meters, the usual height of the lowest layer of cells.

In the LIRAQ model the ground-level emissions affect the average concentration in the grid cell and the shape of the assumed vertical concentration profile that is used to estimate the surface pollutant concentration. The larger the emissions rate, the larger the difference between the calculated surface concentration and the vertical average concentration. Ground-level emissions are injected into the lowest layer of cells in the SAI model. The cells in this layer, as well as all other cells, are assumed to be well mixed at all times. (This is not true of the special microscale layer, which will be described later.) Subsequent to emission, the pollutants are allowed to undergo vertical and horizontal transport, chemical transformations, and removal.

Elevated point source emissions contribute only to the vertical average concentration in the LIRAQ model. To account for the fact that elevated emissions may be injected into the stable inversion layer rather than the mixed layer and that numerical stability problems may be encountered by including sharp temporal changes in the emissions levels injected into a grid cell, MacCracken et al. (1978) designed a special procedure for treating elevated emissions when the mixing depth is relatively shallow. Basically, all elevated source emissions are ignored if the mixing depth is less than 100 meters. The emissions are scaled by a factor that varies smoothly from 0 to 1 as the mixing depth increases from 100 to 150 meters. When the mixing depth is greater than 150 meters, all elevated emissions are injected into the mixed layer. The point source emissions not added to the cell average concentration are ignored in the simulation and cannot be reentrained when the mixing depth rises.

For the SAI model, the height at which the point source emissions are injected is important, since it determines which vertical cell will receive the emissions. Two methods are available for determining this height: The first and easier method is simply to use the stack height; the other method is to determine the plume rise relative to the top of the stack using the Briggs' (1971) formulas, which require the heat flux of the effluents and the local meteorological conditions as inputs. The effective stack height (actual stack height + plume rise) is then used to determine the vertical cell into which the emissions are to be injected. The emissions are completely mixed within this cell and can be transported into adjoining cells according to the winds and turbulent diffusion coefficients. If the effective stack height is higher than the height of the modeling region, then the emissions are not considered further in the simulation.

4. Chemistry

It is not practical to include explicitly within a chemical mechanism all (or a large number) of the hydrocarbon compounds found in an urban atmosphere. Therefore, on the basis of their common properties, the hydrocarbon species must be condensed into a few specific groups. The two most important characteristics used for grouping are reactivity and products formed. The LIRAQ model employs a mechanism similar to that developed by Hecht, Seinfeld, and Dodge (1974), which groups species according to the types of reactions that a compound undergoes in the atmosphere. Three classes of primary species are defined: HC1, which reacts with oxygen atoms, ozone, and hydroxyl radicals and which includes olefins; HC2, which reacts with oxygen atoms and hydroxyl radicals and includes the paraffins and less reactive aromatic species; and HC4, which reacts with oxygen atoms, light, and hydroxyl, peroxyl, and nitrate radicals and which includes aldehydes and ketones. The rates and mechanisms used for these species are representative of propylene for HC1, n-butane for HC2, and a mixture of formaldehyde and acetaldehyde for HC4. HC4 is also a secondary species.

In using the LIRAQ mechanism, it is necessary to distribute the hydrocarbon emissions among the three classes cited above. This can be done using emissions composition data for various source types, as discussed by Duewer (1977). Each type of compound must be assigned to one or more LIRAQ classes. In addition, a factor must be developed to account for the differences in reactivity between a particular compound and those compounds representative of the three LIRAQ groups. This reactivity factor is then used to adjust the hydrocarbon emissions inputs. Thus, reactivity is handled by a complex mixture of species blending and total mass adjustment.

The latest version of the chemical mechanism employed in the SAI model is based on a different approach. The SAI Carbon-Bond Mechanism groups similarly bonded carbon atoms together rather than grouping entire molecules. Six carbon-bond groups are defined: single-bonded, double-bonded (except ethylene), and carbonyl-bonded carbon atoms as well as ethylene, aromatic rings, and benzaldehyde. For example, using this scheme 1 mole of butene would be composed of 2 moles of single-bonded and 1 mole of double-bonded carbon atoms.

The total emissions of all reactive organic compounds are apportioned directly among five of the six carbon-bond classes (no emissions of benzaldehyde are assumed). In contrast to the LIRAQ treatment, no adjustments are made to the mass emissions rates to account for reactivity effects. This is because the Carbon-Bond Mechanism takes advantage of the fact that, when considered on a per carbon atom basis, the range of reactivity of carbon atoms is considerably less than that of hydrocarbon molecules. In addition, because the Carbon-Bond Mechanism follows carbon atoms rather than hydrocarbon molecules, it is possible for the mechanism to maintain a formal mass balance for carbon, a feature that is not an attribute of the LIRAQ mechanism.

The preceding discussion has focused on the treatment of reactions involving organic species to the exclusion of the inorganic reactions. In general, both models treat the important inorganic chemical reactions in about the same amount of detail.

It is important to note that the chemical mechanisms included in the SAI and LIRAQ models are the subjects of ongoing research efforts. As a result, they can be expected to change as new formulations are developed and evaluated. As an example, the SAI mechanism has recently been updated to include six, rather than four, hydrocarbon groups. In addition, this new version of the mechanism includes recent information on the measured values of reaction rate constants and improved treatments of the chemistry of single carbon bonds as well as of aromatic and nitrate compounds.

For some studies, the effect of the previous day's emissions may be of interest. These multiday simulations will necessarily include periods of darkness. The chemical mechanism used for nighttime conditions must recognize the fact that, during periods with no sunlight, the chemistry is no longer driven by the photochemical reactions. Both LIRAQ and the SAI model are at least theoretically capable of treating nighttime chemistry. Basically, the SAI model contains a separate mechanism derived by simplifying the nominal Carbon-Bond Mechanism to reflect only those reactions thought to be important at night. This simplification significantly reduces the amount of computation required to evaluate the reaction rate expressions during the nighttime portion of a simulation. The LIRAQ model employs the same mechanism for both day and night conditions, though different parts of the mechanism are important during each of these periods.

Some difficulties have been experienced in using both the SAI and LIRAQ models to simulate the transition period between daytime and nighttime conditions. During the development stages, the SAI model sometimes predicted negative concentrations during this transition period, but this problem has been virtually eliminated. The numerical method used in the LIRAQ model (a modified Gear routine) can be computationally very slow during a transition period under some conditions. For example, in the St. Louis application, more computer time was required for the period covering sunset than for the entire daylight period. Once the transition period is passed, however, neither model exhibits any further problems.

During daylight hours when the photolysis rates are constantly changing, the LIRAQ model updates each photolysis rate constant for every time step on the basis of the solar zenith angle at that time (each rate constant is independently tabulated versus zenith angle). All the values are adjusted by a transmissivity value for that grid square for that time period. The transmissivity values are derived from Eppley pyranometer data and are a measure of the amount of sunlight reaching the ground to account for clouds, fog, or particulates that may reduce the available sunlight.

The SAI model also updates the photolysis rate constants for every time step but a different procedure is used: The photolysis rates are not all independent; instead, each is defined as the ratio of the particular photolysis rate constant to that for NO_2.* The NO_2 rate is input at the beginning and end of every input data time period. To obtain a value at each time step, the rate constant is determined by linear interpolation within the time period. If aerosols are simulated, then the rate constants are subject to a linear variation with height throughout the column of cells on the basis of the aerosol concentration within the column. This

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* Basically, the SAI model assumes that each photolysis rate constant has the same dependence on the solar zenith angle, though several rate constants are known to exhibit a different dependence from 1 to 2 hours just after sunrise and just before sunset.

procedure accounts for the effects of light scattering due to the presence of aerosols on the available UV radiation in each grid cell. No provision is included for spatially varying the photolysis rate constants to account for clouds or fog in one part of the region but not in another.

Spatial and temporal variations in the photolysis rate constants are treated in more detial in the LIRAQ model than in the present version of the SAI model. In some situations, such as those periods when the zenith angle is close to 90° (at sunrise and sunset) and when the cloud cover over the modeling region is not uniform, this detail may be important.

5. Other Processes

The removal of pollutants at ground level by physical and chemical processes is treated by both models. Surface deposition is calculated in the LIRAQ model by multiplying the deposition velocity by the calculated pollutant concentration at 1 meter above the surface. Although the deposition velocity is only a function of the pollutant (i.e., it is assumed to possess no spatial variability), the ground-level pollutant concentration is dependent on the diffusivity near the surface, which does vary over the modeling region. Basically, the loss of material due to surface sinks affects the value of the predicted ground-level concentration and also influences the cell average concentration.

In the SAI model the rate of deposition depends upon the pollutant concentration in the lowest cell. In contrast to the LIRAQ model, the deposition velocity used by the SAI model is not uniform over the entire grid. Pollutant removal is assumed to take place in two steps--diffusion to the surface followed by absorption, adsorption, or chemical reaction at the surface. The rate of diffusion is calculated from the wind speed, atmospheric stability, and surface roughness for each grid square. The rate of removal for each species at the surface is a nominal value, which is scaled by a

land use factor. This scaling factor is based on surface characteristics; for example, in previous studies thick vegetation has been assumed to result in relatively fast pollutant removal, and concrete has been assumed not to absorb pollutants at all.

The SAI model includes some consideration of the effects of subgrid-scale concentration variations on the reaction rate; there is no corresponding capability in the LIRAQ model at this time. This optional routine, referred to as the microscale module, requires additional input data and is used to account for nonuniform mixing in the lowest layer of cells. It should be noted that this module has only been exercised in a few studies, and thus, its performance characteristics have not been well established.

Near sources of NO, the local ozone is rapidly consumed to form NO_2 until the NO, NO_2, and O_3 come to equilibrium. This subgrid-scale ozone depletion effect is important in the area immediately downwind of the NO source. At the present time, ozone suppression is only treated around roadways. Although considerable effort has been devoted to developing appropriate means for treating ozone suppression in point source NO plumes, these procedures have not been implemented in the SAI model to date. Thus, NO emissions from motor vehicles are allowed to react only with the ambient ozone in the immediate vicinity of the roadway. The microscale routine adjusts the pollutant concentration in the lowest layer, usually 20 meters high, to account for this localized chemistry effect as well as to calculate a measure of the spatial variation of pollutant concentrations within the cell. If this optional module is not exercised, then the lowest layer is assumed to be well mixed, and the chemistry proceeds from this assumption. The assumption that the lowest layer is well mixed allows any NO emitted to react with any ozone in the grid square, thereby reducing the ozone concentration more than it would actually be reduced.

The additional data required for this microscale option are the NO emissions from the major roadways and a factor related to the number of cars operating on the major roadways and their average speed, for each grid square. These data can usually be derived from the information produced by the transportation model used to calculate the mobile source emissions.

6. Numerical Solution Procedures

Since the mass conservation relationships that form the basis for these models cannot be solved analytically, it is necessary to employ numerical techniques to obtain approximate solutions. There are two aspects of the governing equations that are particularly troublesome numerically: the calculation of horizontal advection and the treatment of the chemical reaction term. One of the main drawbacks of the grid modeling approach, as noted by Liu and Seinfeld (1975), is that the horizontal advection portion of the governing equation is difficult to solve accurately.

A first-order finite difference scheme is used in the LIRAQ model to calculate the advective flux between grid cells. In contrast, the SAI model employs the flux-corrected SHASTA* procedure developed by Boris and Book (1973). Tests conducted at SAI have indicated that the SHASTA procedure is a more accurate means of treating horizontal advection (Reynolds et al., 1976; Killus et al., 1977), especially when there are relatively sharp gradients in the concentration field. We note that the SHASTA procedure is used in the LIRAQ-1 model, which is limited to the consideration of pollutants that are inert or those that undergo first-order reactions. Experience reported by Duewer, MacCracken, and Walton (1978) based on actual LIRAQ model applications to San Francisco indicates that the numberical results generated by the two versions of the LIRAQ model that employ the first-order and SHASTA difference schemes, respectively, seem to agree fairly well. Killus et al. (1977) obtained similar results when applying the SAI model to Los Angeles using both a second-order difference scheme and the SHASTA technique. Thus, it can probably be concluded that the SHASTA procedure would be expected to yield more accurate results in those areas on the grid for which horizontal concentration gradients are relatively large. In other areas, the results from the two procedures should not differ substantially.

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* SHASTA is an abbreviation for Sharp and Smooth Transport Algorithm.

To handle the chemical reaction terms, the LIRAQ model employs an LLL-modified version of the numerical method developed by Gear (1971). We note that this technique is frequently used in chemical mechanism development studies and is acknowledged to be a good procedure for solving systems of stiff ordinary differential equations. However, it was not feasible to adapt the more accurate SHASTA treatment of horizontal advection for use in the Gear routine; thus, the simpler first-order difference scheme was used. The reaction terms in the SAI model are integrated by employing a Crank-Nicolson difference scheme. Basically, this scheme yields a set of nonlinear algebraic equations at each time step, which are solved using a Newton iterative procedure. In comparisons involving the Crank-Nicolson and Gear techniques, predicted concentrations generally agreed with one another to within 10 to 15 percent after a few hours of simulation. A major advantage of the method implemented in the SAI model is computational speed. The computing time required by the SAI model for a region segmented into five vertical layers of grid cells is about one-half that required by the LIRAQ model for the same sized two-dimensional grid.

C. MODEL INPUTS

The first step in preparing the input files to a grid model entails the collection and processing of the available aerometric and emissions data as well as other miscellaneous information such as that pertaining to the topography and land use of the area. The form of these data varies widely from one urban area to another. In most cases, the available data require reformatting prior to their use as inputs to the preprocessor programs that create the input files. Both the LIRAQ and SAI models include series of programs that create the appropriate data files in a form suitable for input to each model. The following discussion describes the types of data needed as input for the existing preprocessor programs, the data manipulations that are necessary in addition to any reformatting, and the input data requirements of each model.

Input preparation is more flexible with the SAI model than with the LIRAQ model; in the SAI model, different methods are available for creating the input files, each with different data requirements. The choice of method is determined by the user on the basis of the amount of data available and the general characteristics of the physical and chemical phenomena that influence pollutant concentrations in the region. In general, data preparation procedures should be adapted to the region of interest. The primary objective of this effort is to identify and implement algorithms that make the best possible use of available data and knowledge. The selection of an appropriate algorithm is especially important in situations in which a particular model input is not well characterized by the data. In light of the previous comments, the existing algorithms for preparing model inputs may not represent the best choice for some new application. In such circumstances, more suitable procedures should be developed and implemented in the models.

1. Emissions Inputs

The treatment of ground-level emissions is very similar in both models. Basically, emissions from different sources, such as dry cleaners, gasoline marketing, space heating, and motor vehicle operation, are summed and gridded. In addition, a temporal distribution and hydrocarbon splits must be specified for each source or source category. The primary difference between the two emissions files are the hydrocarbon species.

In the discussion of the chemical mechanism used by each model, it was pointed out that the reactive hydrocarbons have to be apportioned among different classes. The criteria for assigning a molecule to a particular class is quite different for the two models, and the determination of emissions splitting factors requires a good understanding of how organic species are treated in the chemical mechanisms. The actual methods employed for splitting the hydrocarbons for an application range from using average factors for the entire emissions inventory to deriving splits on the basis of detailed hydrocarbon breakdowns for two or more source categories. The amount of disaggregation (by source category) in the emissions inventory and the availability of information with which to derive emissions splits determine how the sources should be lumped into categories.

Individual point sources can be divided into two categories--those that emit pollutants at heights significantly above the surface and those that inject contaminants into the atmosphere at or near the ground. A stack height of 30.5 meters is used as the criteria in the LIRAQ model for deciding whether point source emissions are included in the ground-level or elevated point source category. This height can be easily changed if desired. For the LIRAQ model, the only inputs for the point sources are the location of the source and the emissions of each pollutant. Since the SAI model has multiple layers of grid cells, the height at which the pollutants enter the modeling region is important. Source emissions that are not expected to be injected into grid cells above the surface layer are treated as ground-level sources. For other point sources, the plume rise is calculated and used to allocate emissions on the grid. Therefore, an effective stack height (the actual stack height plus the plume rise relative to the top of the stack), as well as the location and emission rates of each source must be input.

The effective stack height can be specified by the SAI preprocessor program in either of two ways: The simpler method involves inputting the actual stack height and having the program ignore buoyant plume rise calculations; the preferred approach entails inputting both the stack height and other pertinent effluent characteristics to enable the estimation of the effective stack height using the Brigg's (1971) formulas. These formulas require estimates of the heat flux from the stack. The SAI preprocessor routine that calculates the plume rise estimates the heat flux from input values for the exit temperature and flow rate. The stack diameter and velocity can be substituted for the flow rate. Calculation of the plume rise gives a more accurate representation than use of the stack height in determining the place at which the emissions should be injected on the grid. For both models, if the effective stack height is above the top of the modeling region, then the emissions are ignored in subsequent model calculations.

2. Meteorological Inputs

a. Winds

One of the most important tasks of input preparation is creation of the wind field. The data typically available for this task are surface-level wind measurements throughout the region and instantaneous vertical soundings taken at a few locations usually one to three times a day. To prepare wind inputs, the LIRAQ model uses a diagnostic model called MASCON (Dickerson, 1978). The inputs to MASCON are the inversion height data, the wind measurements, and the topography of the region. For the application to San Francisco, additional wind data were synthesized to give a reasonable wind field. Since wind data do not usually exist for every part of the region, judgments must often be made with regard to the way in which wind velocities should be estimated in these areas and whether the calculated velocities are an adequate representation of the expected flow fields. Making such judgments requires experience and a knowledge of the meteorology of the area.

MASCON was developed to provide a self consistent mass flux field for the LIRAQ model. The mass flux into each grid cell is balanced by the outward flux and changes in the mixing depth so that there is no accumulation or depletion of mass within a cell. This is a necessary condition for any wind field to be used in urban-scale air pollution modeling. Another feature of MASCON is the turning of the wind around the topography and channeling of the winds through valleys and mountain passes. The channeling is very important since it determines the ways in which pollutants generated in the urban area will be transported to suburban and rural areas.

SAI has used several methods to construct wind fields for use in the Airshed Model. The appropriate method for use in a given application depends on the topography of the region and the data available. An algorithm developed at SAI by Killus et al. (1977) was tailored for use with the St. Louis Regional Air Pollution Study (RAPS) data base. It is valid only for relatively flat terrain and makes maximum use of the aloft wind data. This method is not appropriate for use in areas where the terrain significantly influences the wind field.

SAI has also developed a three-dimensional diagnostic wind model for use in areas with complex terrain. The basic characteristics of the wind field produced by this wind model, mass consistency and the wind turning around obstacles, are similar to those of MASCON, but the mathematical formulations of the models are quite different. The inputs to the SAI wind model are the surface temperature field, the surface roughness, the elevation for each grid cell, and the wind velocity along the boundaries of the region. The topography and boundary conditions have a dominant influence on the calculated wind field; thermal circulations estimated from the temperature inputs and surface roughness effects have relatively small influences on the wind field. Surface and upper air wind measurements are used to specify the boundary conditions for each level of the wind model. In order to exercise some influence on the wind velocities computed by MASCON, fictitious wind stations and data are sometimes defined and employed in the model. A similar type of control is possible in the SAI wind model by making suitable adjustments to the values of the wind velocities along the boundaries. Again, the modeler must have a good expectation of what a reasonable wind field looks like before adjustments can be made.

In addition to the above approaches, an interpolation routine is also available as part of the SAI data preparation programs. The routine calculates the x- and y-component of the wind velocity for each surface grid square by averaging the observed wind vectors within a specified radius of the grid square. Each measurement is weighted by the inverse of the distance from the grid square to the wind station. This method also lends itself to the use of synthesized wind data as a possible means of rectifying deficiencies in the calculated wind fields resulting from inadequacies in the available data.

The algorithm developed by Killus et al. (1977) and the three-dimensional wind model both calculate a fully three-dimensional wind field. The wind shear predicted by these models depends almost entirely upon the aloft wind data input to the routines. Since there are usually very limited upper air wind data and all the data are instantaneous measurements, care should be

taken when specifying these inputs. The interpolation routine calculates only the surface wind field; therefore, some additional methodology is needed to generate the wind field for the other grid levels of the modeling region. SAI has used several methods including one that produces no wind shear (i.e., the upper level flows are the same as those at the surface) (Reynolds et al., 1973; Anderson et al., 1977) and another that assumes the wind velocity aloft is a function of the calculated local surface wind velocity and some scaling function derived from the available upper air soundings (Reynolds et al., 1979). Since each method was developed for a specific application, we refer the reader to the indicated reports for further details regarding these procedures.

b. Mixing Depths

The depth of the mixed layer directly affects the dilution of emissions and hence has a direct impact on ambient concentrations. The data available for estimating the mixing depth are vertical temperature soundings and surface temperature data. MASCON uses this data along with the wind data to construct the mass-consistent wind and mixing depth field for the LIRAQ model. The winds and mixing depths are linked, and one cannot be changed independently of the other without nullifying the mass-consistency of the wind field.

The SAI model calculates a vertical velocity for each grid cell to satisfy mass conservation. Since this calculation only considers the cell heights and the horizontal wind components in each level of grid cells, the mixing depth inputs for the SAI model can be specified independently of the horizontal wind field inputs. Using the same types of data input to MASCON, the SAI data preparation programs will construct a spatially and temporally varying mixing depth field. We note that the extent to which the changes in the mixing depth are consistent with convergence and divergence effects in the wind field is dependent on the technical features of the preprocessor used to prepare wind and mixing depth inputs to the SAI model.

c. Other Meteorological Inputs

To estimate the ground-level pollutant concentrations from the cell average concentration, the LIRAQ model calculates a vertical profile for each pollutant. Besides the emissions and deposition velocity, another parameter enters into the calculation of the vertical profiles. This parameter is the turbulent diffusivity coefficient near the surface. This coefficient is calculated by MASCON using a procedure proposed by von Karman as explained by Sutton (1953). In general, if the wind speed is high, the vertical mixing is fast, and the vertical profile is relatively flat. At low wind speeds, the diffusivity is smaller, and the resulting concentration profile exhibits a steeper gradient near the surface. The diffusivity coefficient is also used in the SAI model to estimate turbulent transport between vertical layers; however, in that model, this parameter is calculated internally rather than being input from a preprocessor program.

Another variable input to the LIRAQ model, but not to the SAI model, is the atmospheric transmissivity coefficient. This coefficient is a measure of the effect of clouds, aerosol, and atmospheric scattering on the amount of solar radiation that is available for photodissociation reactions. Gridded values of this variable are interpolated from pyranometer station data. We note that the effects of light scattering on the photolysis rate constants are treated internally in the SAI model.

There are also some meteorologically-related data that are input to the SAI model, but not to the LIRAQ model. Chief among these inputs is the top of the modeling region. For the LIRAQ model, the mixing height is also used as the height of the grid cells, whereas the SAI model allows the height of the top of the modeling region to be different from the mixing height. The height of the region can be a function of the mixing depth, can vary according to some other criteria, or can be constant for the entire grid. The choice usually depends on the importance and height of elevated point source emissions, the existence of strata of pollutants within the inversion, and the type of simulation to be performed (i.e., single daylight period or multiple-day run).

Studies in smog chambers indicate that ozone formation is dependent on temperature. This dependence has been quantified by characterizing the temperature dependence of individual reaction rate constants through the use of the Arrhenius relationship. To employ this relationship, it is necessary to input values of the reaction rate constant at some reference temperature and the value of the activation energy for the reaction. Both models include provisions for treating this temperature effect, but the LIRAQ model provides for only one temperature to be input for an entire simulation, whereas the SAI model provides the option of employing a spatially and temporally varying temperature field. Basically, the user must prepare a file containing gridded surface temperature inputs. If a temperature file is not used, then the value of the rate constants at 25°C are employed in the chemistry routine. The gridded surface temperature data are used as an estimate of the temperature throughout each column of grid cells. This process is straightforward, though the addition of synthesized data may be necessary to obtain realistic gridded surface fields, especially if part of the region is covered by a body of water.

The SAI model also requires the values of five variables that are varied temporally but not spatially: the atmospheric pressure, concentration of water vapor (derived from humidity data), temperature gradient above and below the inversion base, and exposure class. The temperature gradients are used in the calculation of the plume rise for large point sources and as an indication of the atmospheric stability of the air above the lower layer of grid cells. These gradients are calculated from the vertical temperature profiles. The exposure class is a measure of the solar insolation, and it is used to calculate the atmospheric stability within the lower layer of cells.

3. Chemistry Inputs

Although the rate constants and activation energy for each nonphotolysis chemical reaction are input to the models, they differ from the other inputs because they are specific to the mechanism rather than dependent upon the region and the date of the simulation. In general, the rate constants are an integral part of the chemical mechanism, and therefore, any single

rate constant should not be updated or changed without analyzing the effect of the change on the overall performance of the entire mechanism at various hydrocarbon and NO_x concentration levels.

The two models differ as to the amount of information used to estimate the photolysis rate constants. The SAI input is the NO_2 photolysis rate constant at set times, usually one-hour intervals. Interpolation is used to calculate the photolysis rate constant at each integration time step, and the other photolysis rate constants are assumed to be proportional to this value. The LIRAQ input files include a table of photolysis rate constants versus the cosine of the zenith angle for all nine of the photodissociation reactions in the LIRAQ mechanism. At each time step, the zenith angle is calculated by the model, and this table is used to obtain the nine photolysis rate constants. This technique produces a more accurate temporal variation of the individual rate constants than does the SAI methodology.

4. Initial Conditions

The pollutant concentrations at the start of a simulation must be input to both grid models. The initial concentration has to be specified for each grid cell and for each species. Local air quality management districts usually monitor the concentrations of NO, NO_2, O_3, CO, and hydrocarbons as well as SO_2 and particulates at times. Their data are usually reported as 1-hour or 24-hour averages. Both models use interpolation procedures and the available monitoring data to derive initial concentration fields for those species for which there are sufficient data.

The schemes used to contruct the initial concentration fields from the measurements are somewhat similar for the LIRAQ model and the Airshed Model. In LIRAQ, the measured surface concentrations at the start of the simulation are converted to vertically averaged values through the use of Eq. (5) on page 6. These average concentration values are then employed in an inverse distance weighted interpolation scheme to calculate the vertically averaged initial

concentration for each grid cell. In the SAI model, the surface observations are used directly in a similar interpolation algorithm to estimate the initial concentrations in each ground-level grid cell.

The SAI model requires the initial concentration at every grid level, but the interpolation routine calculates only surface concentrations. A few options have been included in the data preparation programs for calculating the initial concentrations in grid cells above the surface layer. If desired, a different method can be used for each species. Possibilities include using exactly the same concentrations for the upper layers as for the surface layer, or inputting a vertical profile that is scaled according to the surface concentration or according to the surface concentration and the boundary concentration at the top of the region. The vertical profile can be related to the mixing depth such that the profile will always have the same value at the top of the mixed layer no matter how the height of the mixed layer might vary over the modeling region at the start of the simulation.

An important computational difference between the routines is that the LIRAQ routine uses the boundary conditions as well as the station observations in the interpolation scheme. Other minor differences exist in the actual equations and the treatment of "barriers," such as mountains. Both methods contain provisions for employing synthesized data to supplement the data bases.

Measurements for some pollutants are not always available. Some species, such as SO_2, may not be measured, though they are known to exist in the atmosphere at measurable (but low) concentrations. For these species, initial concentrations are often set to some nominal background level. In addition, ambient measurements for some of the products of photochemical reactions for which there are no standards are rarely available in urban areas. Since most simulations start just before or just after dawn, the initial concentrations of this class of species would be expected to be very low. Zero or near zero (to avoid division by zero) concentrations are used for these species.

5. Boundary Conditions

The boundary conditions* specify the concentration of pollutants in the air entering the modeling region through the side as a result of horizontal advection or through the top of the region as a result of vertical advection and entrainment caused by changes in the region height. The inputs to the SAI model specify time varying boundary concentrations along the region edges and at the top of the region. The concentrations along each boundary are independent; furthermore, it is even possible for the concentrations to vary spatially along a boundary segment if a given situation warrants the increased detail. Measurements taken at locations just inside or outside the region can aid in estimating the boundary values. If no data are available, background concentration levels or some other suitable values can be used. Pollutant concentrations at the top of the region are even harder to estimate, though special field studies are sometimes carried out (such as, in Los Angeles, St. Louis, Denver, and other cities) that yield information pertaining to the pollutant concentrations aloft. Again, if no data are available, one can assume the presence of background levels or some other appropriate values. However, the edge and aloft boundary conditions may be influenced by large upwind sources or an upwind urban area. If this is the case the boundary conditions could have a significant effect on the pollutant concentrations within the modeling region, and an accurate specification of these boundary concentrations is important. The time scale over which the boundary conditions vary is usually an hour, but this time period can be changed to fit each particular application.

The LIRAQ boundary conditions are treated differently. In that model, boundary conditions are established using the following equation:

$$C_B = (C_o{}^2 + \delta^2 C_a{}^2)^{1/2}$$

where C_B is the boundary concentration, C_o is the background concentration, and C_a is the concentration computed by the model for the cell adjacent to the

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* In this section we omit the vertical boundary condition applied at the surface of the models. Basically, emissions, surface uptake, and pollutant transport from the microscale layer (if this option is exercised) are combined to yield a pollutant flux into the lowest layer of grid cells.

boundary. The parameter δ is set to a value between 0 to 1. Both C_0 and δ are specified by the user for each boundary and are held constant throughout the simulation. This technique does not allow the user to specify the diurnal variation of boundary concentration that might be expected if there were large upwind sources outside of the modeling region. Such a situation, which may exist in some eastern cities, could be handled in the SAI model.

We note that if the air is flowing out of the modeling region at some point on the boundary, then each model simply allows the material in the cell adjacent to the boundary to advect out of the region.

6. Other Inputs

The differing model formulations and assumptions lead to different input requirements. This section will discuss those additional inputs that are needed by either the LIRAQ model or the SAI Airshed Model.

The LIRAQ model discounts any emissions from a grid square in which the land is 25 meters above the regionally interpolated inversion height; therefore, the emissions from areas such as mountain tops that break through the inversion base do not affect the pollutant concentrations in the grid cell above that area. (There must be a cell for every grid square, even if the mixing depth is zero. A minimum height of 50 meters is used.) The MASCON program calculates those areas that lie above the mixed layer according to the meteorological inputs and the average elevation of each grid square. These topographic data are contained on the LIRAQ file QGEO, which is calculated from the U.S. Geological Survey tapes or maps for the region. The file QGEO also contains other map data used in the LIRAQ plotting routines, including information pertaining to the shoreline, river courses, political boundaries, and measurement station locations. Topographical data are not input directly to the simulation portion of the SAI model, but if the wind model is used, this information is needed to calculate the wind field. In addition, topographical data are often used in the preparation of mixing depths.

The SAI inputs include an optional file, TERRAIN, which describes two surface characteristics--the surface roughness and a surface deposition factor. The surface deposition factor is a scaling factor representing the ratio of the average surface uptake velocity for a grid square to that of alfalfa. This factor, which is independent of the pollutant, depends upon the relative amounts of vegetation and man-made surfaces in the grid square. For example, trees have been assumed to have a greater capacity for removing pollutants than grasses, and concrete and asphalt have been assumed to have almost no capacity for uptake of pollutants. Both the surface roughness and the deposition factor can be estimated from land use information. If gridded values cannot be estimated for these two variables, then a single value is used for each variable for the entire grid.

D. MODEL OUTPUT

Since the oxidant standard is based on one-hour average concentrations, the models calculate one-hour averages for each hour of the simulation for each species and each grid cell. The instantaneous concentrations at any time are also available, but they are usually employed only for diagnosing problems that have arisen in a simulation. The hourly average concentration grids constitute the basis of all the output options. The simplest form of output, though not the easiest to use, is a printout of the concentrations in grid format as shown in Figure 1. This type of output provides the maximum amount of information regarding the computed ground-level concentration field at each hour.

Comparison of the model predictions with the actual station observations is usually of interest for assessing model performance. The LIRAQ model uses the calculated concentrations within the grid square in which the station is located for the comparison. The SAI model interpolates between the four surface grid cells closest to the station to calculate a predicted concentration for station comparisons. The observed and predicted concentrations can be tabulated by hour or can both be plotted versus time on the same graph. These plots show how well the model reproduces

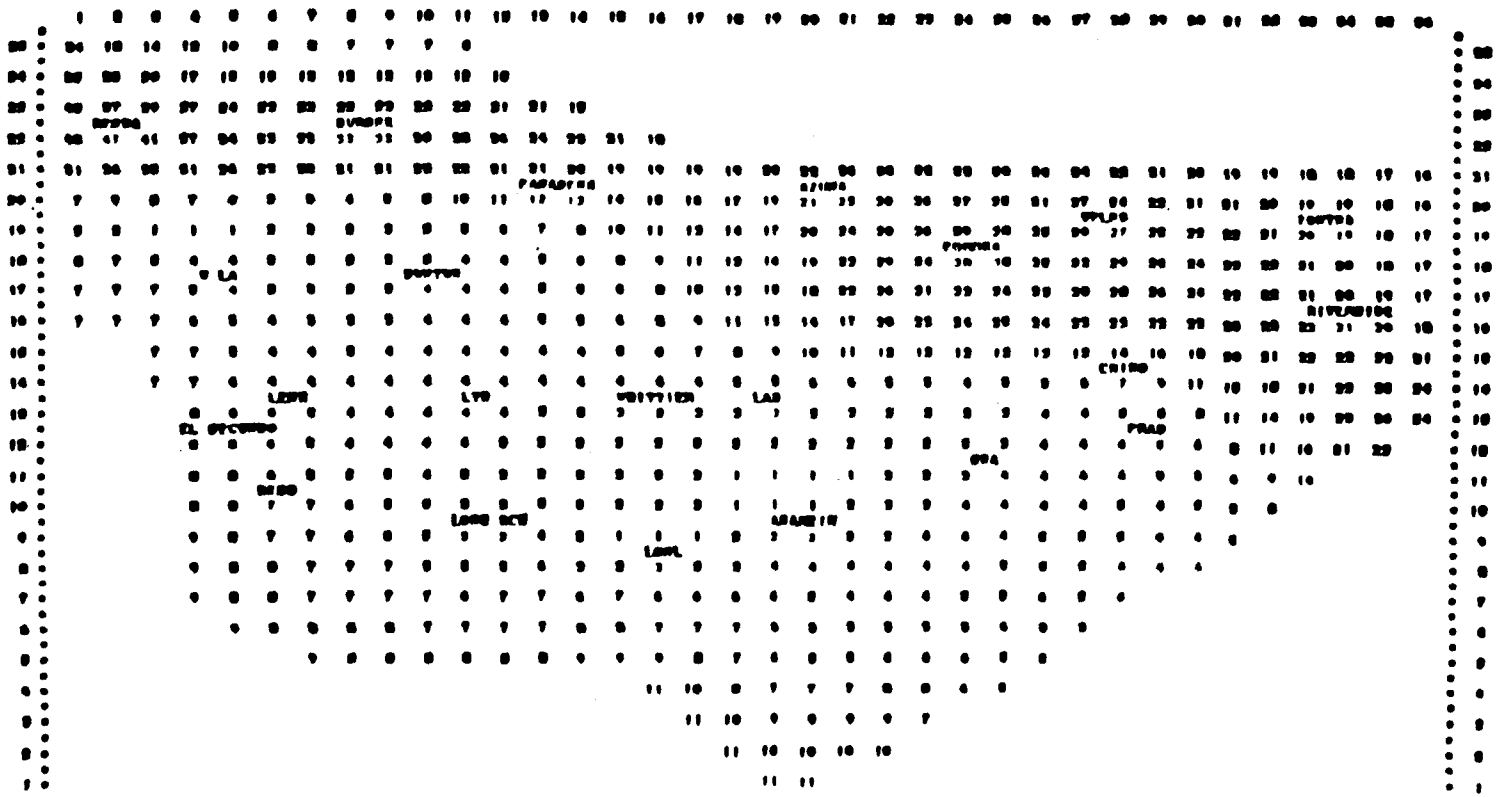


FIGURE 1. EXAMPLE OF A PRINTED MAP OF GROUND LEVEL CONCENTRATION PREDICTIONS PRODUCED BY THE SAI AIRSHED MODEL. Average ground-level O_3 concentrations (pphm) are given for Los Angeles on 4 August 1975 between 1:00 and 2:00 p.m. PST.

the observed diurnal variation of pollutant concentrations and readily indicate any discrepancies between computed and measured values. Such plots can be produced automatically by the LIRAQ model; an example is given in Figure 2.

To quantify further the model's performance, the station observations and predictions can be statistically analyzed. A statistical package is currently available for the LIRAQ model that calculates the mean value, standard deviation, rms error, and the correlation coefficient for the set of observations and predictions at each station.

The most illustrative presentation of the results is isopleth plots. These plots show the regional pattern of the contours of pollutant concentrations with the station locations and other geographical information included for reference. Again, this type of plot can be prepared automatically by the LIRAQ model. Figure 3 is a typical example of one such plot prepared for the San Francisco application.

At the present time, the graphical and statistical programs for displaying the output of the SAI model have not been documented and formally included in the computer codes delivered to the EPA. However, these programs have been employed in previous Airshed Model applications. Examples of station and contour plots are shown in Figures 4 and 5, respectively. In addition, a statistical package is currently being developed by SAI to aid in the analysis of the model results.

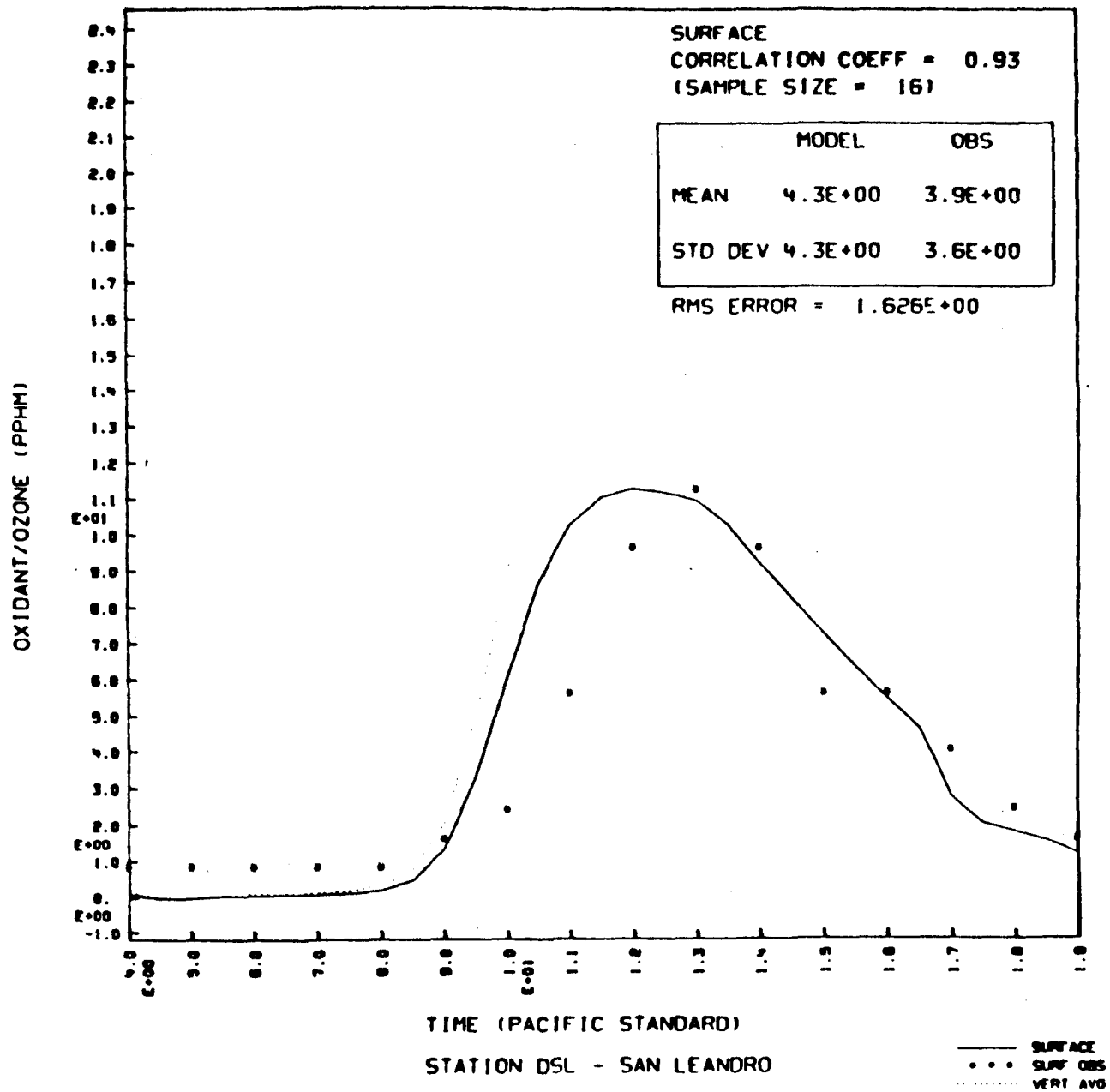


FIGURE 2. AN EXAMPLE OF THE STATION PLOTS PRODUCED BY THE LIRAQ MODEL

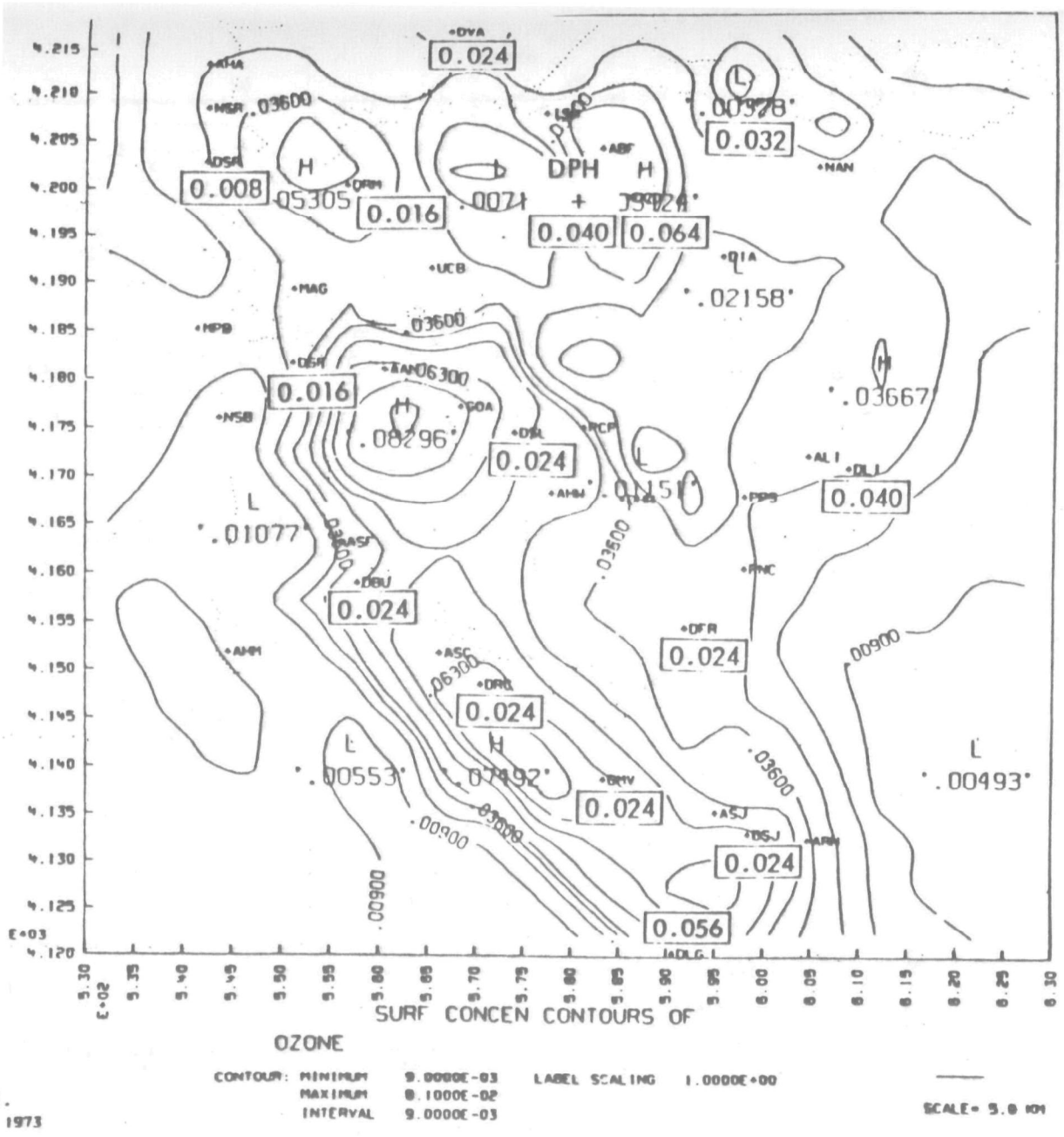


FIGURE 3. AN EXAMPLE OF THE ISOPLETH PLOTS PRODUCED BY THE LIRAQ MODEL. The numbers in the boxes refer to the observed concentrations and have been superimposed on the computer generated graphical output.

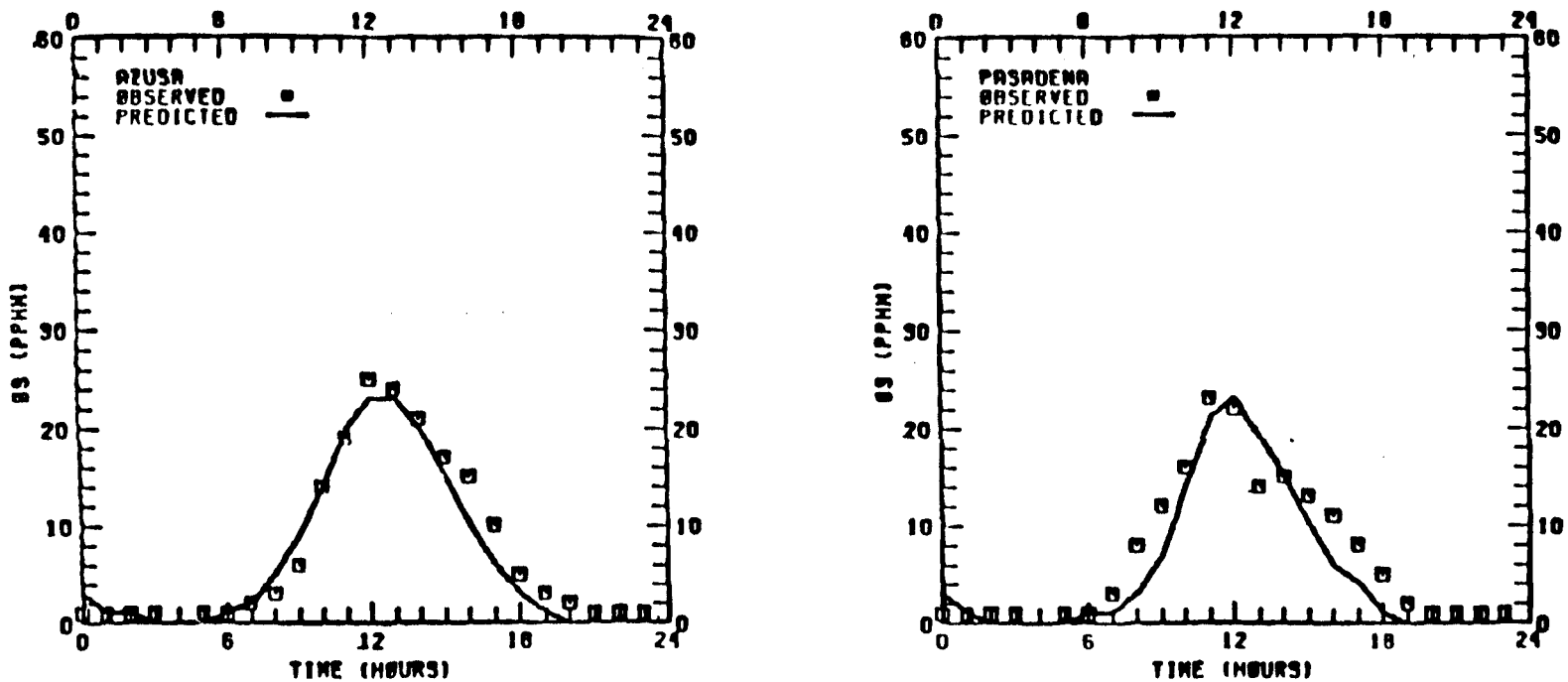
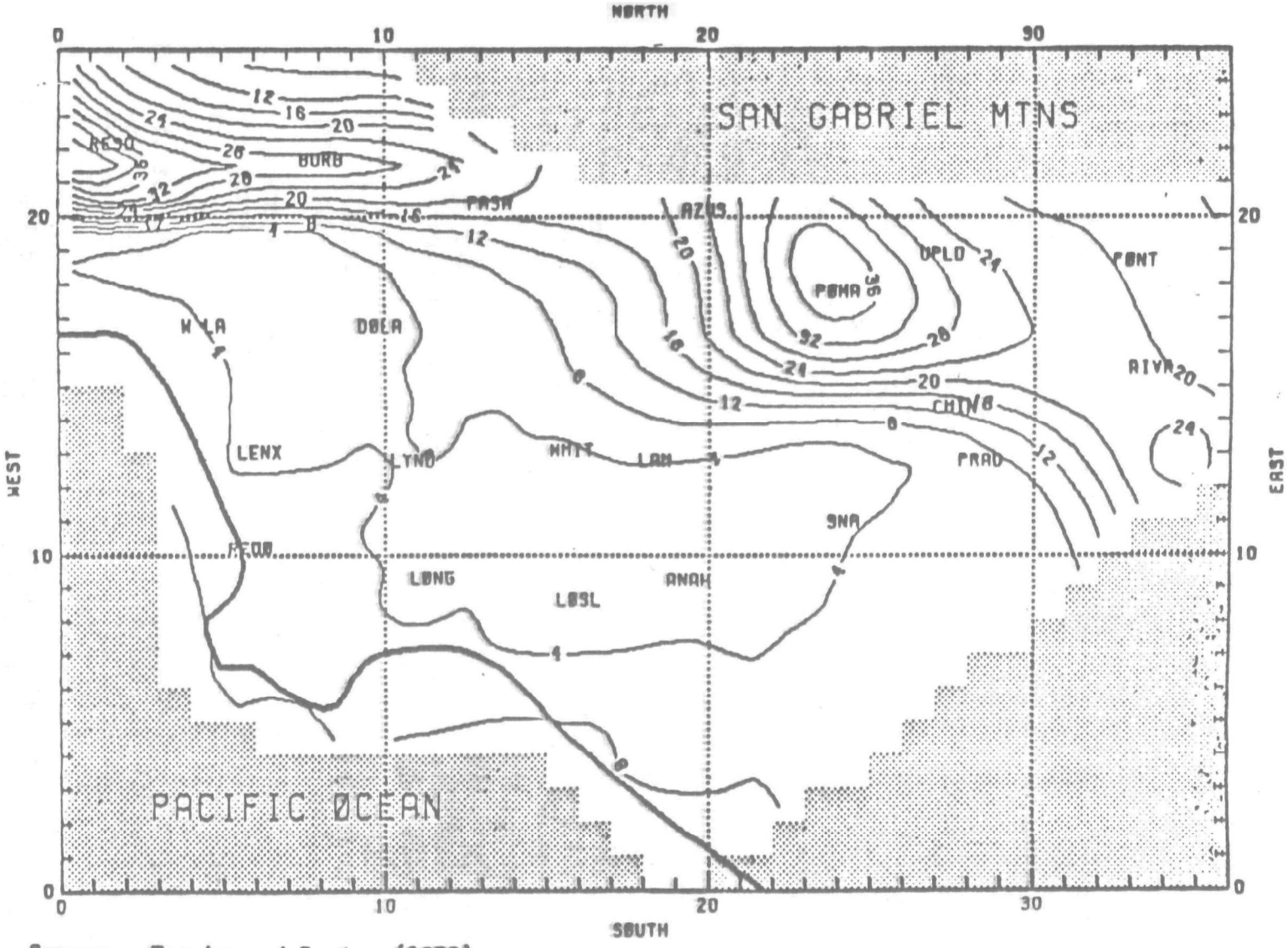


FIGURE 4. EXAMPLE OF PLOTS GENERATED BY THE SAI GRAPHICS PACKAGE ILLUSTRATING COMPUTED AND ACTUAL MEASURED CONCENTRATIONS. Ozone concentrations measured at two stations in the Los Angeles area on 4 August 1975 are compared with the corresponding concentrations calculated by the Airshed Model.



Source: Tesche and Burton (1978).

FIGURE 5. EXAMPLE OF A PLOTTED CONTOUR MAP OF GROUND-LEVEL CONCENTRATION PREDICTIONS PRODUCED BY THE SAI GRAPHICS PACKAGE. Average ground-level O_3 concentrations (pphm) are given for Los Angeles on 4 August 1975 between 1:00 and 2:00 p.m. PST.

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16. ABSTRACT

This document compares the technical features of the SAI Airshed Model with the Livermore Regional Air Quality (LIRAQ) Model. These two state-of-the-art photochemical dispersion models are compared according to their theoretical formulation, components, inputs, and outputs. The model components compared include horizontal transport, vertical transport, emissions, chemistry, and numerical solution procedures.

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