Real-Time Control of Air Pollution

The problem of determining real-time (episode) air pollution control strategies for an urban airshed is posed as selecting those control measures from among all possible such that air quality is maintained at a certain level over a given time period and the total control imposed is minimum. The real-time control is based on meteorological predictions made over a several-hour to several-day period. A computational algorithm is developed for solving the class of control problems that result. The theory is applied to a hypothetical study of the effect of implementation of the optimal control on September 29, 1969, in the Los Angeles basin.

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SCOPE

One of the important environmental problems facing urban officials today is the selection and enforcement of air pollutant emission control measures. These measures take two forms: long-term controls (multi-year legislation, such as the Federal new car emission standards through 1976) and short-term controls (action taken over a period of hours to days to avoid an air pollution episode). What is required for each form of control is a methodology for the systematic determination of the best strategy from among all those possible. The development of a theory for setting long-term controls is in progress (Seinfeld and Kyan, 1971, 1972; Trijonis, 1972). The objective of this paper is the presentation of a theory for the determination of short-term, or real-time, control for urban air pollution.

The determination of real-time controls requires a number of elements: (1) a dynamic mathematical model of atmospheric pollutant concentrations, including meteorological variations and atmospheric chemistry, (2) a contaminant emissions inventory for the airshed, including the temporal and spatial variation of all primary pollutant emissions, (3) an enumeration of all feasible control strategies, and (4) some measure(s) of air quality. Given these elements, the problem is posed as choosing the set of control measures which just maintain air quality and do so at the minimum control level.

Typical control measures include restrictions on the number of motor vehicles allowed on a freeway, reduced operation of power plants, and substitution of low emission fuel (for example, natural gas) for high emission fuel (for example, coal), in power plants. The control strategy is assumed to be enforced over a certain period, say, one hour, based on meteorological predictions made at the beginning of the period. The strategy for each time period could be determined by an air pollution control agency by means of a computer implementing the algorithm presented.

CONCLUSIONS AND SIGNIFICANCE

This paper consists of three parts: (1) the formulation of a general real-time air pollution control problem, (2) the development of a computational algorithm for solving the class of control problems which result, and (3) an application of the theory to a hypothetical study of the effect of implementation of the opimal control on September 29, 1969, in the Los Angeles basin. It is assumed that a mathematical model of pollutant behavior which includes provisions for dynamic meteorology and atmospheric chemical reactions exists for the airshed. The particular type of model utilized for this study consists of an array of well-mixed cells, although the theory is applicable to other types of mathematical air pollution models. Based on the airshed model the real-time control problem is formulated as choosing the types and levels of control actions as a function of time and location in the airshed based on predicted meteorology such that a certain level of air quality is maintained over a given time period and with minimum necessary control action. In the hypothetical study of real-time control for Los Angeles, the pollutant species considered are carbon monoxide, nitric oxide, nitrogen dioxide, reactive hydrocarbons, and ozone. The two control measures assumed to be available were reductions in the number of cars permitted to use freeways and in the amount of fuel burned in the basin's power plants. Various reductions in ozone levels that would have been reached during the day are seen to result from implementation of the optimal strategy. The significance of this paper lies in the framework it provides for the subsequent use of airshed simulation models in control strategy evaluation as such models become available.

Emission control programs for air pollution can be divided into two categories: (1) long-term control, and (2) short-term (or real-time) control. Long-term control strategies involve a legislated set of measures to be adopted by polluting sources over a multi-year period, such as the federal new car exhaust emission standards for carbon

monoxide, nitrogen oxides (NO_x), and hydrocarbons for 1971-1976 new cars. Real-time control, on the other hand, involves emergency measures which are adopted over periods of several hours to several days when expected meteorological conditions are such that an air pollution episode might occur with normal emissions.

A theory for the determination of long-term air pollution control strategies has been presented by Kyan and Seinfeld (1971, 1972). In addition, Kohn (1970, 1972) and Trijonis (1972) have studied the problem of long-term air pollution control. Evaluations of multi-year emission control programs have been carried out for St. Louis (Kohn, 1970, 1972); Farmer, et al., 1970) and Los Angeles (Trijonis, 1972).

Most major cities, however, do not have contingency plans for air pollution emergencies that can be enforced rapidly and unilaterally [an exception is Chicago, a description of whose plan is given by Croke and Booras (1969)]. Also, no work has appeared on the systematic determination of such strategies, including considerations of meteorology, atmospheric chemistry, source strengths and distributions, and available control methods. The development of a general framework for the determination of optimal real-time air pollution control strategies is the object of this work.

First, several points can be noted about the real time problem:

1. This is a dynamic problem in which we are concerned with emissions and pollutant concentrations over time scales of a few hours to a few days;
2. The emergency control measures are in general more severe than emission controls normally in effect and would be only of short duration; and
3. The measures must be capable of being instituted rapidly and effectively.

In principle, a strategy could be designed on the basis of feedback or feedforward control.

In this context, feedback control would imply that we institute control action on the basis of measured atmospheric pollutant concentrations. Thus, we would essentially have to wait until concentrations begin to get serious before taking action, at which time it is usually too late to forestall high concentrations. In general, the tremendous sluggishness of an urban airshed precludes feedback control from being effective.

Feedforward control would imply that we institute control action on the basis of measured meteorological conditions such as wind speed and inversion depth. The distinction between feedback and feedforward control lies in the definition of the system. The airshed is the system, the state of which is the set of pollutant concentrations, the controllable inputs to which are the source emissions, and the uncontrollable inputs to which are the meteorological variables. Feedback control would be based on state (concentration measurements) whereas feedforward control would be based on uncontrollable input (weather factors) measurements. Feedforward control is favorable to feedback control for this problem because we can act before concentrations actually build up. In feedforward control we might, for example, measure wind speeds and inversion depth every few hours as a basis for setting control actions over the ensuing few hours until the next measurements. It is this type of control we will consider here.

We will first briefly discuss the issue of dynamic airshed models, and then develop the general theory of real-time air pollution control. Finally, we present a detailed application of the theory to real time control of carbon monoxide (CO), hydrocarbons (HC), and oxides of nitrogen (NO_x) in the Los Angeles basin.

DYNAMIC AIRSHED MODELS

In order to determine the relationship between emission levels and air quality, a mathematical representation of pollutant behavior in the atmosphere is required. There is currently much interest in the mathematical modeling of urban air pollution. A general survey of the subject has been presented by Seinfeld et al. (1972), and studies (of varying approaches and degrees of success) on modeling specific urban areas are found in Lamb and Neiburger (1971), Randerson (1970), Eschenroeder and Martinez (1971), Roth et al. (1971), and Reynolds, et al. (1973). Most of these studies are based on the numerical solution of some form of the partial differential equations of continuity for the mean concentrations of pollutant species in a turbulent fluid. Because this approach to air pollution modeling is still in a state of development, we have chosen to employ a somewhat simpler model here. We do this primarily to facilitate our real objective in the present work, namely the study of real-time control. Therefore, the airshed model to be used may not ultimately be the most desirable but, nevertheless, is a conceptually simple one which includes provisions for sources, meteorology, and chemistry.

The model we will employ is based on dividing the airshed into an array of well-mixed cells (Ulbrich, 1968; Reiquam, 1970; Seinfeld and Kyan, 1971; MacCracken et al., 1971). Assume the airshed has been divided into an array of K cells, each of which is considered as a well-mixed reactor. The volumes of the cells which need not be equal or constant are $v_1, \ldots, v_K$. The mean concentration of species i in cell j is x_{ij}. Theoretically, this mean concentration is an ensemble mean concentration which results from an average over a very large number of repetitions of identical experiments. In each cell there is a time-varying source of each pollutant E_{ij}. Also, there exists the possibility that pollutants can be formed or depleted by chemical reaction at a rate r_i, or removed by deposition, at a rate d_i. Finally, the volumetric rate of airflow from cell j to cell k is q_{jk}.

A dynamic material balance for species i in cell k is

$$\frac{d}{dt}(x_{ik}v_k) = \sum_{j=0}^{K} q_{jk}\,x_{ij} - x_{ik}\sum_{j=0}^{K} q_{kj} + E_{ik} - d_i + r_i \tag{1}$$

$$x_{ik}(t_0) = x^0{}_{ik} \tag{2}$$

Normally, dv_k/dt is set equal to $a_k(dH_k/dt)$, where a_k is the area of the base of a cell having vertical sides and H_k is the height of the base of an inversion or a convenient mixing depth. In effect, the cell is a box with permeable walls and a movable lid. The subscript zero on q_{kj} and x_{ij} refers to flows into and out of the airshed. Subsequently we will neglect deposition, as we will consider only gaseous pollutants.

For conciseness we express (1) and (2) in vector notation as

$$\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t) + \mathbf{B}(t)\mathbf{b}(t) + \mathbf{r}(\mathbf{x}) + \mathbf{E}\mathbf{u} \tag{3}$$

$$\mathbf{x}(t_0) = \mathbf{x}^0 \tag{4}$$

where $\mathbf{x}(t)$ is the NK-dimensional column vector, $[x_{11}, x_{12}, \ldots, x_{1K}, x_{21}, \ldots, x_{NK}]^T$, and the $NK \times NK$ matrix

$$\mathbf{A} = \begin{bmatrix} \mathbf{D}^T & & & 0 \\ & \mathbf{D}^T & & \\ & & \ddots & \\ 0 & & & \mathbf{D}^T \end{bmatrix} \tag{5}$$

where the $K \times K$ matrix

$$\mathbf{D} = \begin{bmatrix} -\frac{1}{v_1}\left(\dot{v}_1 + \sum_0^K q_{1j}\right) & \frac{q_{12}}{v_2} & \cdots & \frac{q_{1K}}{v_K} \\ \frac{q_{21}}{v_1} & & & \\ \vdots & & & \\ \frac{q_{K1}}{v_1} & \cdots & -\frac{1}{v_K}\left(\dot{v}_K + \sum_0^K q_{Kj}\right) & \end{bmatrix} \tag{6}$$

Also, the $NK \times NK$ matrix

$$\mathbf{B} = \begin{bmatrix} \mathbf{P} & & 0 \\ & \mathbf{P} & \\ & & \mathbf{P} \\ 0 & & \end{bmatrix} \tag{7}$$

where the $K \times K$ matrix

$$\mathbf{P} = \begin{bmatrix} \frac{q_{01}}{v_1} & & 0 \\ & \frac{q_{02}}{v_2} & \\ & & \frac{q_{0K}}{v_K} \end{bmatrix} \tag{8}$$

$\mathbf{b}$ is an NK-dimensional vector of pollutant concentrations outside the airshed, $[x_{10}, x_{10}, \ldots, x_{10}, x_{20}, \ldots, x_{20}, \ldots, x_{N0}, \ldots, x_{N0}]^T$, $\mathbf{r}(\mathbf{x})$ is an NK-dimensional vector of reaction rates, $\mathbf{u}$ is an NK-dimensional vector of the mass emissions of the N pollutants in each of the K cells (that is, if we let e_{nk} be the mass emissions of pollutant n per hour in cell k, then $\mathbf{u} = [e_{11}, e_{12}, \ldots, e_{1K}, e_{21}, e_{22}, \ldots, e_{2K}, \ldots, e_{NK}]^T \equiv [u_1, u_2, \ldots, u_{NK}]_T$, where $u_{(n-1)K+k} \equiv e_{nk}$), and $\mathbf{E}$ is an $NK \times NK$ matrix required to convert the emissions (mass/time) into concentrations (ppm/time).

STATEMENT OF THE PROBLEM

The problem we wish to solve is the following: Given a meteorological forecast from time t_0 to time t_f, determine the set of control measures applied to polluting sources over (t_0, t_f) such that a given set of air quality criteria are not violated and the amount of required emission reduction is a minimum.

The meteorological parameters in the airshed model are $\mathbf{A}(t)$, $\mathbf{B}(t)$, $\mathbf{b}$ and any that may occur in $\mathbf{r}(\mathbf{x})$, such as the temperature or intensity of radiation. Thus, at time t_0 measurements of wind speeds and directions, inversion heights, temperatures, etc. are assumed to be available. On the basis of these measurements, $\mathbf{A}(t)$, $\mathbf{B}(t)$, $\mathbf{b}$, etc. are forecasted over (t_0, t_f) so that henceforth we will assume these quantities are given. A reasonable duration for the predictions would be two hours.

A general measure of air quality at any time is some prescribed function $\mathbf{g}(\mathbf{x})$. For example, if air quality is given by the concentration of species 1 in each of the K cells, then $\mathbf{g}(\mathbf{x})$ is simply equal to $[x_{11}, x_{12}, \ldots, x_{1K}]^T$. The maximum allowable value of g can be called $\mathbf{g}^*$.

Pollutant emissions enter the airshed model through $\mathbf{u}(t)$, the mass emissions of each contaminant in each cell as a function of time. The uncontrolled level of emission can be denoted by $\mathbf{u}_0(t)$. We could pose the real-time control problem as minimizing some measure of the deviation between the normal level of emissions $\mathbf{u}_0(t)$ and that needed for control $\mathbf{u}(t)$ subject to (3)-(8) and $\mathbf{g}(\mathbf{x}) \leq \mathbf{g}^*$.

As stated, this problem will yield the maximum allowable mass emission levels, $u_1(t), \ldots, u_{NK}(t)$, over the time interval (t_0, t_f), needed to maintain a certain air quality index $\mathbf{g}^*$, given meteorological information over the interval, that is, $\mathbf{A}(t)$, $\mathbf{B}(t)$ and $\mathbf{b}$. The solution to this problem will not, however, tell us what controls to impose —it only tells us what maximum mass emission levels e_{nk} of each pollutant in each cell can be tolerated while still maintaining $\mathbf{g}(\mathbf{x})$ below $\mathbf{g}^*$. We have no guarantee that these mass emission levels can, in fact, be reached in the necessary proportions with existing control methods. This is a key point in what follows. The reason is that the emission reductions of various primary pollutants achieved with any control method are not independent. For example, an automobile emits carbon monoxide, hydrocarbons, and oxides of nitrogen in certain relative proportions dependent on the age of the car, its condition, etc. These emissions cannot be altered independently by the types of strategies available for real-time control, such as reducing freeway traffic; a change in the driving patterns in an area will affect all emissions in a fixed manner. For this reason, it is necessary to consider as control variables not simply the total mass emissions $\mathbf{u}(t)$ but rather the level of employment of the actual control methods. For example, u_{11} might represent the mass emissions of CO (species 1) in cell 1. This value is a result perhaps of a number of control methods acting on several sources of CO in cell 1. Merely determining u_{11} will not tell us either how to achieve that value of u_{11} or, in fact, even if that value is attainable given existing control methods. We must therefore enumerate the feasible control methods for each source, as well as all the important sources in the airshed.

In order to include information relating to the sources and their controls we introduce the following definitions:

- p = number of source types in the airshed (for example, 1970 motor vehicles, power plants, etc.)
- q_i = number of control methods available for source i, $i = 1, 2, \ldots, p$.
- s_{ik} = magnitude of source i in cell k (for example, the number of 1970 motor vehicles in cell k) $i = 1, 2, \ldots, p$; $k = 1, 2, \ldots, K$.
- d_{ijk} = level of control activity j on source type i in cell k (for example, the number of 1970 motor vehicles prohibited from freeway use in cell k) $j = 1, 2, \ldots, q_i$; $i = 1, 2, \ldots, p$; $k = 1, 2, \ldots, K$.
- r_{ijn} = the reduction in the mass emission of pollutant n by application of one unit of control method j for source i (for example, the pounds/hr of CO reduced per 1970 motor vehicle prevented from freeway use in cell k) $j = 1, 2, \ldots, q_i$; $i = 1, 2, \ldots, p$; $n = 1, 2, \ldots, N$.
- ω_{ij} = the number of units of source i controlled by one unit of control method j (for example, $\omega_{11} = 1$ if one 1970 car is prevented from freeway use).

Therefore, the d_{ijk} are the variables which represent the level of source control by each model. We assume that the parameters above can be taken as constants independent of the level of control.

We can now relate the overall mass emissions u_l, $l =$

$(n-1)K+k$, to the individual sources and their controls by

$$u_{l_0} - u_l = \sum_{i=1}^{p} \sum_{j=1}^{q_i} r_{ijn}\, d_{ijk}\, s_{ik}, \quad l = (n-1)K + k \tag{9}$$

$$n = 1, 2, \ldots, N$$

$$k = 1, 2, \ldots, K$$

where, as we noted previously, u_{l_0} is the uncontrolled level of emission. (9) may be expressed somewhat more concisely as

$$\mathbf{u} = \mathbf{u}_0 - \mathbf{G}\mathbf{w} \tag{10}$$

where $\mathbf{G}$ is a NK by $K \cdot \Sigma q_i$ matrix

$$\mathbf{G} = \begin{bmatrix} \boldsymbol{\Gamma}(1) \\ \boldsymbol{\Gamma}(2) \\ \cdot \\ \cdot \\ \cdot \\ \boldsymbol{\Gamma}(N) \end{bmatrix} \tag{11}$$

with the K by $K \cdot \Sigma q_i$ matrix $\boldsymbol{\Gamma}(n)$ given by

$$\boldsymbol{\Gamma}(n) = \begin{bmatrix} \boldsymbol{\nu}_n(1) & & & 0 \\ & \boldsymbol{\nu}_n(2) & & \\ & & \cdot & \\ & & \cdot & \\ 0 & & & \boldsymbol{\nu}_n(K) \end{bmatrix} \quad n = 1, \ldots, N \tag{12}$$

where the Σq_i-dimensional row vector $\boldsymbol{\nu}_n(k)$ is

$$\boldsymbol{\nu}_n(k) = [r_{11n}s_{1k}, r_{12n}s_{1k}, \ldots, r_{1q_1n}s_{1k}; \ldots; r_{p1n}s_{pk}, \ldots, r_{pq_pn}s_{pk}]$$

$$k = 1, \ldots, K$$

$$n = 1, \ldots, N$$

The $K \cdot \Sigma q_i$ dimensional vector $\mathbf{w}$ is defined by

$$\mathbf{w} = [\mathbf{h}^T(1), \mathbf{h}^T(r), \ldots, \mathbf{h}^T(K)]^T$$

where the Σq_i dimensional vector $\mathbf{h}(k)$ is

$$\mathbf{h}(k) = [d_{11k}, d_{12k}, \ldots, d_{1q_1K}; d_{21k}, \ldots, d_{2q_2k}; \ldots; d_{p1k} \ldots d_{pq_pk}]^T$$

We can write (3) as

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{b} + \mathbf{r}(\mathbf{x}) + \mathbf{E}(\mathbf{u}_0 - \mathbf{G}\mathbf{w}) \tag{13}$$

Thus (13) is our new airshed model equation, and $\mathbf{w}$ is our new control vector. Our objective will be to determine $\mathbf{w}$ over the interval (t_0, t_f).

To simplify the problem somewhat, we make the follow-two assumptions:

1. The matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{b}$ and $\mathbf{E}$ are constant over the interval (t_0, t_f). In other words, once a set of meteorological measurements are made at t_0, conditions are assumed to be constant until t_f, when presumably a new set of measurements are made. As noted before, reasonable value of $t_f - t_0$ might be two hours.

2. The control actions $\mathbf{w}$ are constant over (t_0, t_f). (Since control strategies will involve actions such as reducing freeway traffic or power plant operations, it is impractical to update the strategy too frequently, so this is an entirely reasonable requirement.)

We choose as the explicit form of the air quality constraint $\mathbf{g}(\mathbf{x}) \leq \mathbf{g}^*$,

$$\Psi(\mathbf{x}(t_f)) + \int_{t_0}^{t_f} \varphi(\mathbf{x}(t))\, dt \leq 0 \tag{14}$$

The two terms account for the instantaneous concentrations at the end of the control period t_f and dosages during the entire control period, respectively. Although we do not include explicitly a constraint on concentrations over the whole control period, appropriate choice of Ψ and φ will serve to keep concentrations below a desired level.

The individual control variables d_{ijk} must satisfy two constraints, namely that

1. the number of source units controlled not exceed the total source units

$$\sum_{j=1}^{q_i} \omega_{ij}\, d_{ijk} \leq s_{ik} \quad i = 1, 2, \ldots, p \tag{15}$$

2. the number of control units be non-negative

$$d_{ijk} \geq 0 \tag{16}$$

Finally, we must specify the objective function to be minimized. We have stated that we desire to minimize the deviation between normal emission levels and those required to meet the air quality criteria. Perhaps a better choice would seem to be to minimize the total cost of control rather than simply the amount of reduction required. However, costs associated with a certain measure are often not easy to estimate. This is particularly true in the case of real-time controls, such as rerouting of traffic or providing only limited access to freeways. Consequently, we will not consider costs as our objective function, although control costs are almost always closely tied to the level of control required, so that omission of explicit costs is not a serious drawback in the problem formulation.

A reasonable choice for the objective function is the quadratic form, $J = \mathbf{w}^T\mathbf{Q}\mathbf{w}$, where $\mathbf{Q}$ is a pre-specified weighting matrix. If no control is applied $J = 0$, since, by definition, $\mathbf{w} = 0$. Thus, we want to keep J as close to zero as possible.

In summary, the general problem to be solved is the following: Minimize J with respect to $\mathbf{w}$, subject to the constraints, (13) and (14) to (16). In the next section we develop a computational method to solve this problem.

GENERAL METHOD OF SOLUTION

Since $\mathbf{w}$ is a set of constant parameters, the general problem is a mathematical programming problem with both nonlinear and differential equation constraints. We now present a computational method for determining $\mathbf{w}$ which minimizes J subject to the constraints above. The method is based on iterative improvement of an initial guess $\mathbf{w}^{(0)}$. We begin by linearizing (13) about a nominal control $\mathbf{w}^{(0)}$ and the corresponding nominal trajectory $\mathbf{x}^{(0)}$. The perturbation $\delta\mathbf{x} = \mathbf{x}(t) - \mathbf{x}^{(0)}(t)$ is governed by

$$\delta\dot{\mathbf{x}}(t) = [\mathbf{A} + \mathbf{r}_{\mathbf{x}}(\mathbf{x}^{(0)}(t))]\, \delta\mathbf{x} - \mathbf{E}\mathbf{G}\delta\mathbf{w} \tag{17}$$

$$\delta\mathbf{x}(t_0) = 0 \tag{18}$$

where $\delta\mathbf{w} = \mathbf{w} - \mathbf{w}^{(0)}$. We wish to choose the increment $\delta\mathbf{w}$ such that J is minimized and (14) to (16) are satisfied,

$$\Psi[\mathbf{x}^{(0)}(t_f) + \delta\mathbf{x}(t_f)] + \int_{t_0}^{t_f} \varphi[\mathbf{x}^{(0)}(t) + \delta\mathbf{x}(t)]\, dt \leq 0 \tag{19}$$

$$\mathbf{Z}\,\delta\mathbf{w} \leq \mathbf{y} - \mathbf{Z}\mathbf{w}^{(0)} \tag{20}$$

$$-\delta\mathbf{w} \leq \mathbf{w}^{(0)} \tag{21}$$

where $\mathbf{y}$ is the pK-dimensional column vector $[s_{11}, s_{21}, \ldots, s_{p1}, s_{12}, s_{22}, \ldots, s_{p2}, \ldots, s_{pK}]^T$ and the K-dimensional block-diagonal matrix

$$\mathbf{Z} = \begin{bmatrix} \mathbf{W} & & 0 \\ & \mathbf{W} & \\ & & \ddots \\ 0 & & \mathbf{W} \end{bmatrix} \tag{22}$$

where $\mathbf{W}$ is the $p \times \Sigma q_i$ matrix

$$\mathbf{W} = \begin{bmatrix} \boldsymbol{\mu}(1) & & 0 \\ & \boldsymbol{\mu}(2) & \\ & & \ddots \\ 0 & & \boldsymbol{\mu}(p) \end{bmatrix} \tag{23}$$

and $\boldsymbol{\mu}(i)$ is the q_i-dimensional row vector $[\omega_{i1}, \omega_{i2}, \ldots, \omega_{iq_i}]$.

In order to obtain (19) in a form amenable to computation, we linearize the constraint about $x^{(0)}(t)$,

$$\Psi(\mathbf{x}^{(0)}(t_f)) + \Psi_{\mathbf{x}}(\mathbf{x}^{(0)}(t_f))\,\delta\mathbf{x}(t_f) + \int_{t_0}^{t_f} [\varphi(\mathbf{x}^{(0)}(t)) + \varphi_{\mathbf{x}}(\mathbf{x}^{(0)}(t))\,\delta\mathbf{x}(t)]\,dt \leq 0 \tag{24}$$

The solution of (17), a set of linear differential equations with time-varying coefficients (that is, $\mathbf{r}_{\mathbf{x}}(\mathbf{x}_0(t))$) can be expressed as

$$\delta\mathbf{x}(t) = -\int_{t_0}^{t} \boldsymbol{\Phi}(t, \tau)\,\mathbf{EG}\delta\mathbf{w}\,d\tau \tag{25}$$

where the $NK \times NK$ transition matrix $\boldsymbol{\Phi}(t, \tau)$ satisfies

$$\frac{\partial \boldsymbol{\Phi}(t, \tau)}{\partial t} = [\mathbf{A} + \mathbf{r}_{\mathbf{x}}(\mathbf{x}^{(0)}(t))]\,\boldsymbol{\Phi}(t, \tau) \tag{26}$$

$$\boldsymbol{\Phi}(\tau, \tau) = \mathbf{I} \tag{27}$$

Using (25), (24) becomes

$$[\Psi_{\mathbf{x}}(\mathbf{x}^{(0)}(t_f))\,\mathbf{FEG} + \mathbf{VEG}]\,\delta\mathbf{w} \geq \Psi(\mathbf{x}^{(0)}(t_f)) + \int_{t_0}^{t_f} \varphi(\mathbf{x}^{(0)}(t))\,dt \tag{28}$$

where

$$\mathbf{F} = \int_{t_0}^{t_f} \boldsymbol{\Phi}(t_f, \tau)\,d\tau \tag{29}$$

and

$$\mathbf{V} = \int_{t_0}^{t_f} \varphi_{\mathbf{x}}(\mathbf{x}^{(0)}(t')) \int_{t_0}^{t'} \boldsymbol{\Phi}(t', \tau)\,dt'\,d\tau \tag{30}$$

Thus, the problem of determining $\mathbf{w}$ can be stated as follows:

$$\underset{\delta\mathbf{w}}{\text{Min}}\, J = \underset{\delta\mathbf{w}}{\text{Min}}\, \{\delta\mathbf{w}^T\,\mathbf{Q}\,\mathbf{w}^{(0)}\} \tag{31}$$

subject to (20), (21), and (28). Since δJ [the right-hand side of (31)] and the constraints (20), (21), and (28) are linear in $\delta\mathbf{w}$, this problem can be solved by linear programming.

We note the $\boldsymbol{\Phi}(t, \tau)$ is not explicitly required in this problem, rather only the integral (29) given by $\mathbf{F}$. By inspection we see that

$$-\int_{t_0}^{t} \boldsymbol{\Phi}(t, \tau)\,d\tau\,\mathbf{EG} = \frac{\partial \mathbf{x}}{\partial \mathbf{w}} \tag{32}$$

where $\partial\mathbf{x}/\partial\mathbf{w}$ is the $NK \times NK$ matrix of sensitivity coefficients of the state $\mathbf{x}$ to the control $\mathbf{w}$. Thus, $\boldsymbol{\Phi}$ need not be evaluated explicitly. The sensitivity matrix can be computed by perturbing $\mathbf{w}^{(0)}$ by $\mathbf{w}^{(0)} + \boldsymbol{\epsilon}$ and computing by finite differences

$$\frac{\partial x_i}{\partial w_j} \cong \frac{x_i(t) - x_i^{(0)}(t)}{\epsilon_j} \tag{33}$$

The computational scheme is as follows:

1. Choose a nominal control $\mathbf{w}^{(0)}$ and solve (13) to obtain the nominal state $\mathbf{x}^{(0)}(t)$. A convenient initial guess $\mathbf{w}^{(0)}$ is the uncontrolled emission level $\mathbf{w} = 0$.
2. Evaluate $\mathbf{F}$ and $\mathbf{V}$ by the procedure described in conjunction with (32) and (33). The perturbations $\boldsymbol{\epsilon}$ are arbitrary and are not necessarily related to $\delta\mathbf{w}$.
3. Determine $\delta\mathbf{w}$ by minimizing (31) subject to (20), (21), and (28) by linear programming. Compute the next iterate of $\mathbf{w}$ by $\mathbf{w}^{(1)} = \mathbf{w}^{(0)} + \delta\mathbf{w}$. Return to step 1 with $\mathbf{w}^{(1)}$ in place of $\mathbf{w}^{(0)}$.
4. When $|J(\mathbf{w}^{(m+1)}) - J(\mathbf{w}^{(m)})|/J(\mathbf{w}^{(m)})$ is less than a certain criterion, stop.

REAL-TIME CONTROL OF PHOTOCHEMICAL SMOG IN THE LOS ANGELES BASIN

As an application of the general theory we have developed, we will consider real-time control of air pollution in the Los Angeles basin. The results to be presented should be viewed only as preliminary with respect to a final control scheme for Los Angeles. The primary reason is that the well-mixed cell airshed model that we will employ here is rather crude compared to a model currently being developed based on the continuity equations for mean concentrations of the pollutant species (Roth et al., 1971). Thus, the evaluation of the real-time control method is the principal aim of this section as opposed to the presentation of a validated mathematical model for photochemical smog in Los Angeles. The latter study is available (Reynolds et al., 1973).

Figure 1 presents a map of the Los Angeles basin with a 2-mile × 2-mile-grid overlaying a 50-mile × 50-mile area. The locations of major sources as well as the Los

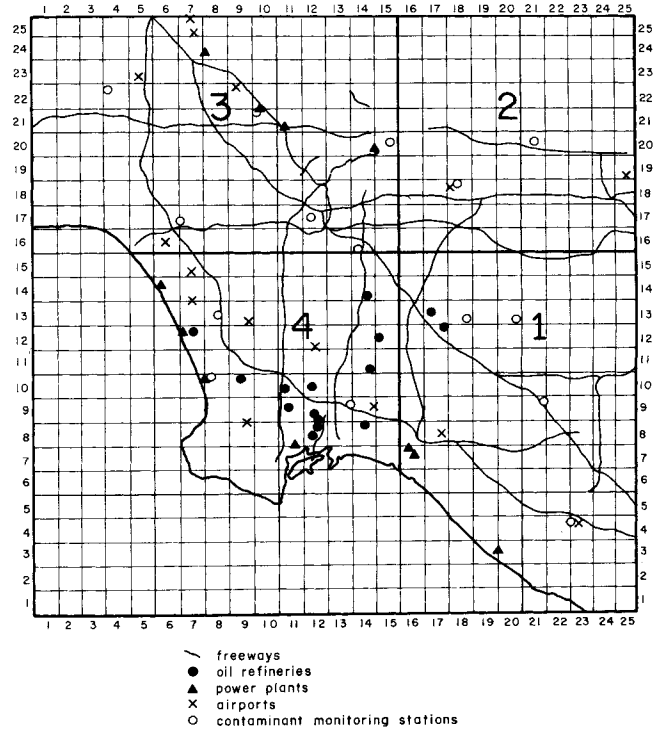

Fig. 1. Location of primary sources and monitoring stations in the Los Angeles Basin.

Angeles County Air Pollution Control District (APCD) pollutant monitoring sites are shown. The primary pollutants of most importance in Los Angeles are CO, NO_x, and hydrocarbons, with SO_2 and particulate matter of somewhat less importance. The most significant secondary pollutants (those formed in the atmosphere by chemical reaction) are NO_2 and O_3. It is well established that the major sources of primary pollutants in Los Angeles are motor vehicles and power plants, with smaller contributions from refineries, industrial operations, and aircraft (Lemke, 1971). Prevailing wind patterns are essentially the same in summer and winter, that is, from the west to the east.

The behavior of the various species varies with summer and winter conditions. CO distributions (due entirely to motor vehicles) are approximately the same all year, except that early morning winter concentrations are higher than summer. NO concentrations are highest in early morning in the vicinity of freeways and power plants. NO_2, which is not emitted in significant quantities from sources, is formed in the atmosphere by oxidation of NO, and subsequently converted to nitric acid and organic nitrates in the photochemical smog reactions. NO_2 concentrations are higher in the winter, when, because of shorter days and less intense sunlight, the photochemical reaction sequence does not proceed to completion. In summer, on the other hand, the primary NO and hydrocarbons react to completion to yield large quantities of O_3, as the air parcels traverse the basin from west to east.

Our real-time control study will center on summer time conditions, since it is in the summer that the typical Los Angeles smog is felt to be most damaging, primarily because of the high ozone concentrations achieved. We will consider the following species: CO, NO, hydrocarbons (HC), NO_2 and O_3. The first three are primary pollutants, while the latter two are secondary pollutants. We neglect SO_2 and particulate matter because control measures in effect in Los Angeles have reduced these two pollutants to considerably lesser importance than CO, NO, and hydrocarbons. For our exercise we have chosen a typical day in 1969, namely September 29, on which pollutants concentrations were reasonably high. What we will examine, therefore, is the effect that real-time controls would have had if they had been imposed on that day.

As the sources amenable to control we have selected for this study freeway motor vehicle traffic and power plant operations. We exclude surface street motor vehicle traffic because of the difficulty of its control. In each case, a partial reduction in the source activity is chosen as the control measure, that is, reducing the number of vehicles allowed on freeways and reducing the amount of fuel burned (power delivered) in certain power plants. The control strategies will depend on the location of the sources as well as their uncontrolled hourly emission rates.

The question of the practicality of these control measures is a central one. In view of the nature of the Los Angeles air pollution problem, real-time control actions must certainly focus on motor vehicle traffic and perhaps to a somewhat lesser extent on power plant operations. With respect to motor vehicle traffic, the question then is —what is an effective means of reducing traffic and still providing the means for people to get to work? We will not attempt to answer this question here, although a system currently under study, involving appreciably expanded use of buses on special freeway lanes, is a realistic approach. Because of the size of and the freeway patterns in Los Angeles, it is unlikely that, in the face of restricted freeway traffic, a large number of people would elect surface street routes as opposed to available mass transit.

We will require several items to be able to carry out the control exercise, namely,

1. An emissions inventory for CO, NO, and HC in the Los Angeles basin for 1969. This inventory will provide information on the location and hourly emissions from all major sources of these contaminants.
2. A kinetic mechanism for the atmospheric chemical reactions involving CO, NO, NO_2, HC and O_3. This will provide the functional form of $\mathbf{r}(\mathbf{x})$.
3. Meteorological data, including hourly averaged wind speeds and directions and inversion depths, for the area to be modeled on September 29, 1969.

Clearly, these elements are required for the validation of any mathematical model of urban air pollution. As we noted above, our primary intent here is to test and examine the theory developed for real-time control rather than to formulate and validate an air pollution model. Consequently, we will not dwell too extensively on the comparison of the predictions of the well-mixed cell model with actual monitoring data.

EMISSIONS INVENTORY FOR THE LOS ANGELES BASIN

The major sources of pollutant emissions in an airshed may be classified as moving and fixed. The predominant moving source in all urban airsheds is vehicular traffic, primarily automobiles and trucks, with smaller contributions coming from aircraft. Power plants, refineries, and industrial operations are the principal fixed sources of pollutants in the Los Angeles basin.

There is a multiplicity of models for pollutant emissions that may be applied to individual sources and source types. The model that is used, and the degree of detail that is incorporated, is dependent upon the spatial and temporal resolution of the overall airshed model, the type and amount of data available, and the accuracy of those data. For example, in attempting to estimate contours of pollution concentrations over the Los Angeles basin during the course of a day and under particular meteorological conditions, it is necessary to compute the distribution over space of pollutant emissions from automobiles with a resolution of the order of one mile, and over time with a resolution of the order of one hour.

A motor vehicle emissions inventory can be divided into two parts: (1) estimation of spatial and temporal distribution of traffic; and (2) estimation of average vehicle emission rates applicable to traffic in the area. The spatial and temporal distribution of traffic on the freeways and surface streets in an urban area can be estimated from traffic counts which are normally taken by state and local agencies. Vehicle exhaust emissions rates are estimated from data collected in tests that simulate the emissions of vehicles actually driven over typical routes in the urban area being studied.

Data for the motor vehicle emissions inventory for Los Angeles for 1969 have been compiled by Roberts et al. (1971, 1972). In this study the spatial distribution of motor vehicle traffic was obtained from the traffic counts of freeways and major and minor street intersections and compiled for each of the 625 2-mile × 2-mile-grid squares shown in Figure 1. Figure 2 shows the geographical distribution of freeway traffic in the Los Angeles basin in 1969 in thousands of vehicle miles/day as determined by Roberts et al. (1971). A similar distribution, not presented here, was compiled for surface street traffic. The temporal distribution of both freeway and surface street traffic was determined by traffic count information and is shown in Figure 3. The freeway distribution was derived from 15-min. traffic count data over a 24-hour period at 31 freeway locations, while the surface street distribution was compiled from traffic counts on 52

randomly selected city streets.

The emission rates of CO, NO, and HC were based on the computation of emissions for an average vehicle in 1969 based on the distribution of vehicle ages, makes, and sizes in the Los Angeles basin and on the federal driving cycle as representative of an average trip. Details of the computation are presented by Roberts et al. (1971, 1972). Resulting emission rates are given in Table 1.

There are 11 power plants in the Los Angeles basin, the locations of which are indicated in Figure 1. Data relating to locations, capacities, and emissions are published annually by the Los Angeles County APCD (for example, Lemke, 1971). It was assumed that total daily power plant emissions are distributed equally over the 24-hour period. Average emission rates applicable to 1969 appear in Table 1. (In the computations, account was taken of the fact that each particular plant may vary in its emission characteristics.)

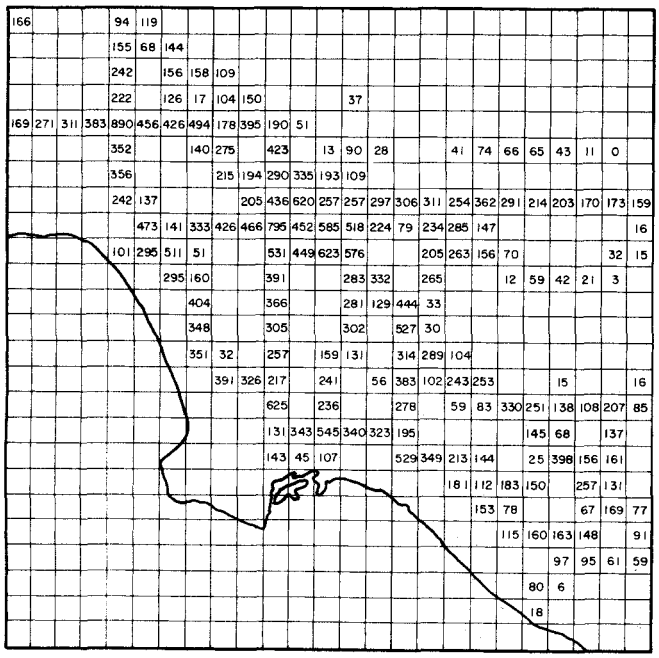

Fig. 2. Geographical distribution of freeway traffic in the Los Angeles Basin in late 1969 (thousand vehicle miles per day)

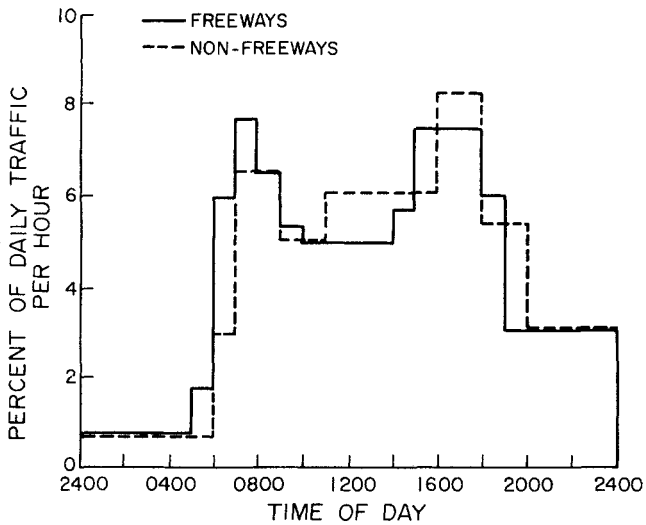

Fig. 3. Temporal distribution of freeway and surface street motor vehicle traffic in the Los Angeles Basin in late 1969.

TABLE 1. AVERAGE EMISSION RATES FROM MOTOR VEHICLES AND POWER PLANTS IN 1969

	CO	NO	HC
Motor vehicles	63.9 g./mile	2.726 g./mile*	7.66 g./mile
Power plants	0.0	544.42 g./mwhr.**	0.0

* NO_2 emissions assumed to be 0.13 grams/mi.
** NO_2 emissions assumed to be 35.86 g./mwhr.

TABLE 2. SPATIAL DISTRIBUTION OF MAJOR SOURCES IN THE LOS ANGELES BASIN IN 1969 IN THE FOUR CELLS SHOWN IN FIGURE 1

Sources	Cell 1	2	3	4
Freeway motor vehicles, 10^6 miles/day	9.765	4.245	19.19	8.595
Surface motor vehicles, 10^6 miles/day	16.5	7.368	27.31	21.105
Power plants, mw	4410	0	1069	3217

Subsequently we shall consider two control cases: (1) CO control only, and (2) CO, NO, and HC control. Because of the large dimensionality in the latter case ($N = 5$) when all five species are considered, computing time requirements force us to employ only a four-cell model. The four regions bounded by the heavy lines in Figure 1 constitute the four cells. The spatial distribution of major sources in the four cells is summarized in Table 2. In the case of CO control only, however, since only a single species is involved, it is possible to use a model with considerably more cells. Thus, we let $K = 20$ in the CO control case, as used previously by Kyan and Seinfeld (1972). We do not illustrate the 20 cells here.

KINETIC MECHANISM FOR PHOTOCHEMICAL SMOG

The reaction term $\mathbf{r}(\mathbf{x})$ accounts for the rate of production of each species by chemical reaction in the atmosphere and depends in general on the concentrations of each of the n species. There will be instances in which the use of an airshed model will be limited to the prediction of concentrations of inert species. However, when chemical reaction processes are of importance, it is essential to include an adequate description of these phenomena in the model.

A discussion of the development of kinetic mechanisms for photochemical smog suitable for inclusion in an airshed model would take us too far afield. Reviews of smog chemistry can be found in Altshuller and Bufalini (1971) and Johnston et al. (1970). A generalized kinetic mechanisms for photochemical smog that has been successful in simulating both laboratory and atmospheric data is that of Hecht and Seinfeld (1972). The mechanism, together with values of the kinetic parameters used in this study, is given in Table 3. Differential equations are required for NO, NO_2, O_3, and HC (the generalized hydrocarbon species), while the other species are assumed to be in a pseudosteady state. To conserve space, we do not present the explicit form of $\mathbf{r}(\mathbf{x})$ here. These may be found in Seinfeld et al. (1971).

METEOROLOGICAL DATA

The required meteorological data for implementation of the model are the intercell flow rates q_{jk} and the cell volumes v_k as a function of time. The intercell flow rates

can be obtained from wind fields, whereas inversion heights are necessary to compute v_k. Wind speeds and directions as a function of time and location have been prepared by Roth et al. (1971) based on hourly-averaged surface wind data at 34 stations in the Los Angeles basin on September 29, 1969. Inversion heights were estimated based on measured vertical temperature profiles at three stations on the same day. Contours of constant inversion height were constructed on hourly maps by assuming the contours to be roughly parallel to the coastline. Inversion heights for the entire basin were then interpolated from the three contours.

The wind data in Roth et al. (1971) were resolved into east-west and north-south components and the appropriately summed and averaged to produce the hourly q_{jk} required for the four cells. Inversion height data were used to give the cell heights H_k. Table 4 presents a typical set of this data for 11 a.m.

We have noted that our object here is not to present a validated mathematical model for Los Angeles air pollution; such a study is available (Reynolds et al 1973). Nevertheless, it is useful to have some idea of the validity of the cell model employed here. Since the cells are so large, particularly in the case of K = 4, it is not particularly revealing to compare the readings at one station to the average values in a 100-sq. mi. region in which the station is located. However, as an indication of the concentration levels and temporal trends of both the actual data and the model, we present Figures 4 and 5. Figure 4 shows the NO concentration simulated for cell 4 and the measured values at two stations in cell 4, Long Beach and Lennox. Figure 5 shows a similar comparison for O_3 in cell 3 and measurements at the Reseda station in cell 3. Also shown in Figure 5 is the average O_3 concentration at all stations in cell 3.

TABLE 3. KINETIC MECHANISM FOR PHOTOCHEMICAL SMOG*

	Reaction	Rate constant employed
1.	$NO_2 + h\nu \rightarrow NO + O$	22.2 hr^{-1}‡
2.	$O + O_2 + M \rightarrow O_3 + M$	1.656×10^8 hr^{-1} (pseudo first order)
3.	$O_3 + NO \rightarrow NO_2 + O_2$	1.308×10^3 ppm^{-1} $hr.^{-1}$
4.	$O_3 + 2NO_2 \xrightarrow{H_2O} 2HNO_3$	0.36 ppm^{-1} hr^{-1}**
5.	$NO + NO_2 \xrightarrow{H_2O} 2HNO_2$	0.24 ppm^{-1} $hr.^{-1}$
6.	$HO_2\cdot + NO_2 \rightarrow HNO_2 + O_2$	600 ppm^{-1} $hr.^{-1}$
7.	$HNO_2 + h\nu \rightarrow OH\cdot + NO$	0.3 $hr.^{-1}$‡
8.	$CO + OH\cdot \xrightarrow{O_2} HO_2\cdot + CO_2$	1.2×10^4 ppm^{-1} $hr.^{-1}$
9.	$HC + O \rightarrow \alpha RO_2\cdot$	1.2×10^5 ppm^{-1} $hr.^{-1}$, $\alpha = 2.7$
10.	$HC + O_3 \rightarrow \beta RO_2\cdot + RCHO$	0.06 ppm^{-1} $hr.^{-1}$, $\beta = 0.5$
11.	$HC + OH\cdot \rightarrow \delta RO_2\cdot$	3.6×10^5 ppm^{-1} $hr.^{-1}$, $\delta = 1.2$
12.	$RO_2\cdot + NO \rightarrow NO_2 + \epsilon OH\cdot$	1.08×10^5 ppm^{-1} $hr.^{-1}$, $\epsilon = 0.6$
13.	$RO_2\cdot + NO_2 \rightarrow PAN$	600 ppm^{-1} $hr.^{-1}$
14.	$HO_2\cdot + NO \rightarrow NO_2 + OH\cdot$	1.08×10^5 ppm^{-1} hr^{-1}

* Reference–Hecht and Seinfeld (1972).

** Reaction 4 is a composite of the three reactions.

$$O_3 + NO_2 \rightarrow NO_3 + O_2$$
$$NO_3 + NO_2 \rightarrow N_2O_5$$
$$N_2O_5 + H_2O \rightarrow 2HNO_3$$

‡ k_1 and k_7 depend on the light intensity and are related to the time in Los Angeles by

$$\frac{k_i(t)}{k_{i\,max}} = 1.017 - 0.06846\left(\frac{t-12}{6}\right) - 1.0764\left(\frac{t-12}{6}\right)^2 \quad i = 1,7$$

where t is the time in hours ($t = 12$ is noon) and $k_{i\,max}$ is the value given above.

TABLE 4. INTERCELL FLOWS q_{jk} AND CELL VOLUMES v_k AT 11 A.M. FOR THE FOUR CELLS SHOWN IN FIGURE 1

	$q_{jk} \times 10^{-10}$ cu. m./hr.				
j	0	1	2	3	4
k					
0		1.193	0	1.024	3.922
1	2.199	0	0.684	0	0
2	1.459	0	0	0	0
3	2.052	0	0.775	0	0.465
4	0.429	1.69	0	2.268	0
v_k, $m^3 \times 10^{-10}$		4.053	2.573	7.013	4.736

CONTROL PARAMETERS

The source types we consider amendable to control are freeway motor vehicle traffic and fuel consumption in power plants ($p = 2$). For each of the two source types the sole control method is a reduction in the source activity ($q_1 = q_2 = 1$). Thus, (9), (15), and (16) reduce to

$$\sum_{i=1}^{2} r_{i1n}\, d_{i1k}\, s_{ik} = e_{nk0} - e_{nk} \qquad \begin{matrix} n = 1, 2, \ldots, 5 \\ k = 1, 2, 3, 4 \end{matrix} \tag{34}$$

and

$$0 \leq d_{ik} \leq 1 \qquad \begin{matrix} i = 1, 2, \\ k = 1, 2, 3, 4 \end{matrix} \tag{35}$$

where the control parameters are defined as follows:

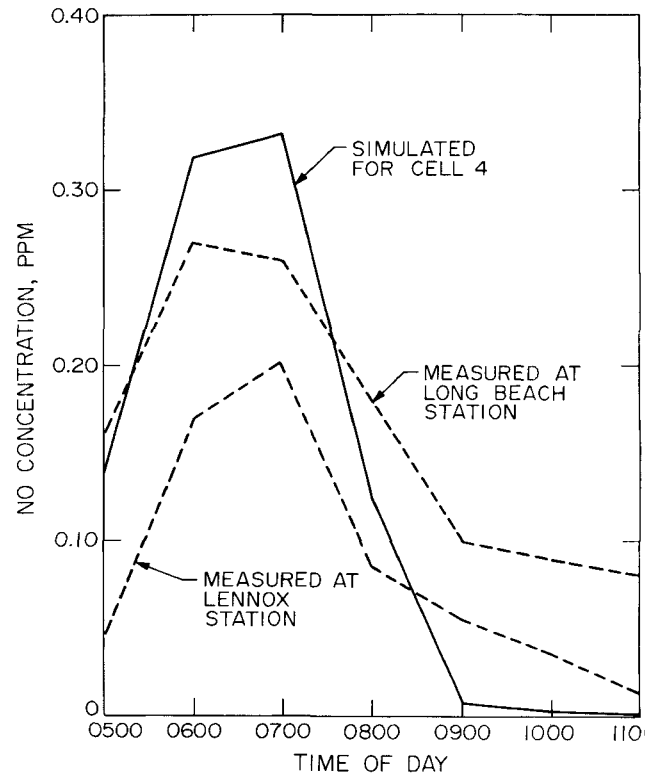

Fig. 4. Simulated NO concentration in Cell 4 and measured NO concentrations at Long Beach and Lennox Monitoring Stations in Cell 4.

TABLE 5. CONTROL POLICY FOR THE CO CASE, EXPRESSED AS FRACTIONAL REDUCTION IN FREEWAY MOTOR VEHICLE TRAFFIC

Hour	Cell no. 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
5-6 a.m.				0.11	0.56			0.06	0.08										0.54	0.57
6-7 a.m.			0.56						1.0	0.75		0.75	0.74	0.75	0.71	0.69	0.47			0.16
7-8 a.m.					0.31				0.29			0.78	0.79							
8-9 a.m.														0.01						

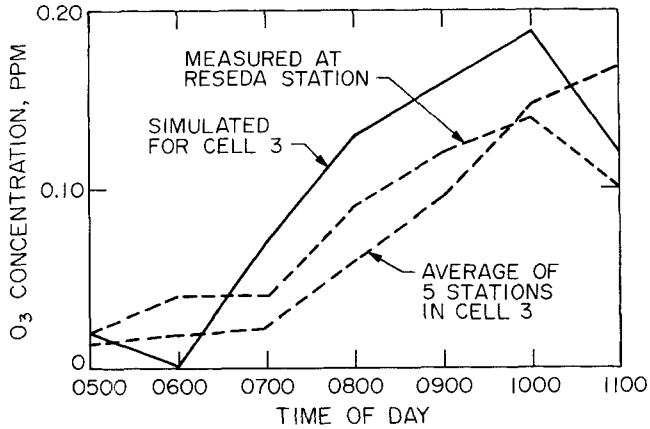

Fig. 5. Simulated O_3 concentration in Cell 3, measured O_3 concentration at Reseda monitoring station, and average of O_3 concentrations measured at 5 stations in cell 3.

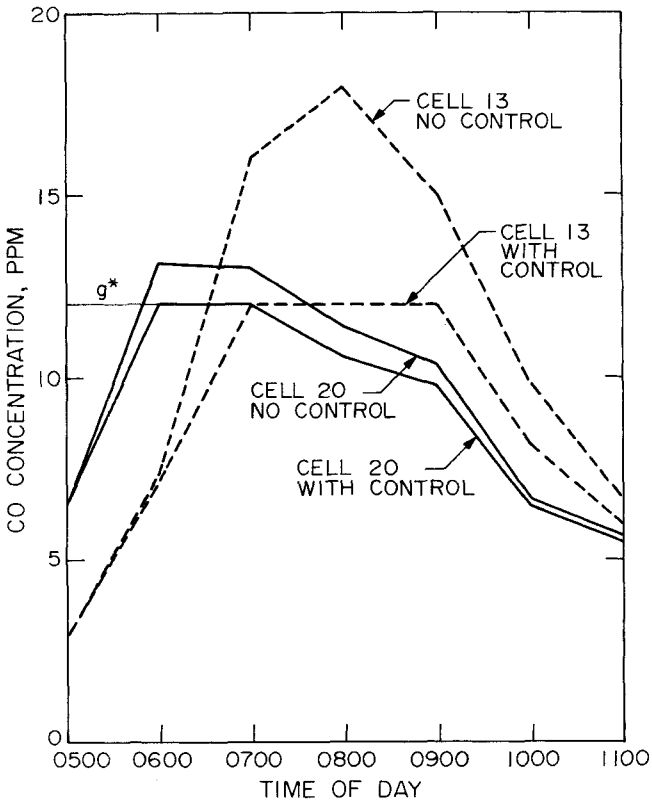

Fig. 6. Comparison of uncontrolled CO concentrations with those resulting from real-time control in cells 13 and 20 (20-cell simulation).

r_{11n} = reduction in emissions of species n (grams) per motor vehicle mile reduction below normal level. See Table 1.

r_{21n} = reduction in emissions of species n (grams) per megawatt reduction in power plant output below normal level (equal to zero for all pollutants but NO and NO_2). See Table 1.

d_{11k} = fractional reduction in freeway mileage in cell k during time period (t_0, t_f).

d_{21k} = fractional reduction in megawatt output in cell k during time period (t_0, t_f).

s_{1k} = normal vehicle miles travelled on freeways in cell k during (t_0, t_f). See Table 2.

s_{2k} = normal megawatts delivered in cell k during (t_0, t_f). See Table 2.

CONTROL RESULTS

Figure 6 shows the results of implementation of the real-time control strategy for only CO in cells 13 and 20. The air quality constraint employed is $x_i(t_f) \leq 12$ ppm, $i = 1, 2, \ldots, 20$, that is, that at the end of the control period (one hour) that the CO concentration in any cell not exceed 12 ppm. Only values of concentrations at the end of each hour were assumed to be reported, and these values are connected by straight lines in Figure 6 and subsequent figures. Table 5 shows the temporal and spatial reductions in freeway traffic needed to achieve the results in Figure 6. Major reductions in freeway traffic are called for during the period 6 to 8 a.m. in central Los Angeles and the San Fernando Valley.

Figure 7 presents a comparison of ozone concentrations in cells 1 and 3 with and without real-time control. The air quality constraints employed were that the ozone concentrations at the end of the control period (5 hours) not exceed 0.29 and 0.13 ppm in cells 1 and 3, respectively. A control period of 5 hours (5 to 10 a.m.) was chosen in the NO_x, HC, O_3 case because the secondary pollutant O_3 resulting from early morning emissions attains its peak values several hours after the early morning rush hour. Therefore, it is necessary to choose a control period long enough to see the effect of the control of early morning emissions. Different air quality constraints were chosen primarily to illustrate the flexibility of the theory.

Table 6 shows the spatial distribution of reductions in both freeway traffic and power plant operations during the period 5-10 a.m.

DISCUSSION

The objective of this study has been the formulation and testing of a framework for considering real-time air pollution control strategies. The key aspects are the proper definition of the real-time control problem with respect to an airshed model and its solution rather than the advocacy of any particular model. Since, as we have noted, the well-mixed cell airshed model will probably

Table 6. Control Policy for Photochemical Case Expressed as Fractional Reduction of the Freeway Traffic and Power Plant Operations

Hour		Cell 1	2	3	4
5-10 a.m.	freeway traffic	0.67	0.0	0.45	0.77
	power plants	0.57	0.0	1.0	0.0

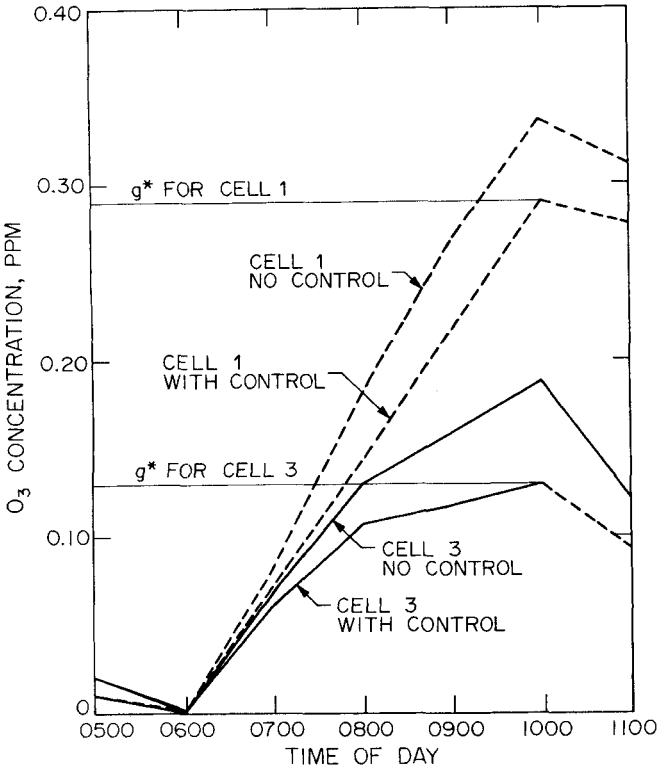

Fig. 7. Comparison of uncontrolled O_3 concentrations with those resulting from real-time control in cells 1 and 3 (4-cell simulation).

not be the form employed in the future for large urban simulations, but rather one based on the partial differential equations for the mean concentrations of pollutants [the so-called "semi-empirical equation of atmospheric diffusion" (Monin and Yaglom, 1971)], an important question to which we must address ourselves here is—can the theory we have presented be implemented with feasible computing requirements on the more complex models to come?

When dealing with the control of essentially inert pollutants, such as CO, particulate matter, and SO_2 (which for control purposes can be considered inert), we feel the answer is yes. The computing storage and time requirements for the 20 cell CO control exercise for Los Angeles were quite modest (70,000 bytes of storage, 40 sec. for 8-hr. control on an IBM 370/155). Both the storage and time requirements would increase proportionately with the number of grid squares used in the model for single pollutant control.

Although we have illustrated the theory in a case of chemically reacting air pollution in order to show its application under the most general circumstances, at this time it appears that extension to a model consisting of coupled, three-dimensional partial differential equations, while theoretically feasible, is not practical given current computing capabilities. For example, the 4-cell Los Angeles exercise involving 5 species required storage of 220,000 bytes and 10 min. of computing time for the 8-hour control results in Table 5. Extension to 5 coupled partial differential equations on a 427 × 5 mesh with $\Delta t = 5$ minutes, as reported by Reynolds et al. (1973) would require more than one hour of computing for a comparable control exercise. As with similar problems, such as global weather simulation, mathematical modeling of chemically reacting urban air pollution will require considerable computing capacities, thereby making control exercises an expensive (but necessary) undertaking.

ACKNOWLEDGMENT

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Separations via Semicontinuous Parametric Pumping

A semicontinuous parametric pump with batch operation during one half-cycle and continuous operation in the other half-cycle was experimentally investigated using the model system toluene-*n*-heptane on silica gel adsorbent. A mathematical model based on an equilibrium theory is presented and is found to be in good agreement with the experimental results. Furthermore, it is shown that when the penetration distance for the cold cycle is less than or equal to that of the hot cycle and the height of the column, the rate of production of pure solvent by this pump may become quite large compared to the rate of production by a pump in which operation is continuous during both half-cycles.

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SCOPE

Parametric pumping is a phase-change separation process which depends for its operation on the coupling of periodic changes in some variable affecting the position of interphase equilibrium with synchronous periodic changes in flow direction. As first investigated by Wilhelm and Sweed (1968), the variable, temperature, was used to change the equilibrium distribution of toluene between a toluene-*n*-heptane solution and a bed of silica gel adsorbent particles. In reservoirs attached to the ends of the beds, separation factors (defined as the ratio of toluene concentrations in the two reservoirs) as high as 10^5 were attained after a relatively small number of cycles of up- and downflow accompanied by synchronous temperature changes. This high separation capability provided an incentive for the development of mathematical models which could predict separations and possibly a basis for commercial design.

Pigford et al. (1969) originated an important and simple equilibrium theory and, based on the theory, derived mathematical expressions for the performance of the batch parametric pump (Wilhelm and Sweed, 1968). Two primary assumptions of the theory were those of instantaneous local equilibrium throughout the adsorption column and absence of axial diffusion. Later, Aris (1969) showed that the theory of Pigford et al. is a special case of a more general theory and derived the general theory.

By extending the equilibrium theory, Chen and Hill (1971a) have derived mathematical expressions for the performance of batch, continuous, and semicontinuous parametric pumps. Their continuous pump, characterized by a steady flow for both feed and product streams during the upflow and downflow cycles, has a truly continuous operation in nature. On the other hand, the semicontinuous pump is operated batch-wise during upflow and continuously during downflow. They have shown that under certain conditions the batch pump and the continuous and semicontinuous pumps with feed at the enriched end have the capacity for complete removal of solute from one product stream and, at the same time, give arbitrarily large enrichment of solute in the other product stream. Recently Chen et al. (1972) verified the models and analytical solutions for the continuous pump in the model system toluene-*n*-heptane on the silica gel adsorbent. The experimental values compared reasonably well with the calculated results.

In the present paper, a semicontinuous pump with top feed is experimentally investigated using the model system of toluene-*n*-heptane on silica gel adsorbent. A comparison is made between the experimental data and the analytical results based on the equilibrium theory. Emphasis is given to the operating conditions required to obtain higher production rates of pure solvent for the semicontinuous pump as compared to the continuous pump.

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