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The GEOMET Indoor-Outdoor Air Pollution Model

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THE GEOMET INDOOR-OUTDOOR AIR POLLUTION MODEL

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ABSTRACT

This report documents the formulation of the GEOMET Indoor-Outdoor Air Pollution (GIOAP) model. The model estimates indoor air pollutant concentrations as a function of outdoor pollutant levels, indoor pollutant generation sources rates, pollutant chemical decay rates, and air exchange rates. Topics discussed include basic principles, model formulation, parameter estimation, model statistical validation, and model sensitivity to perturbations of the input parameters.

The numerical estimates obtained from the GIOAP simulations have been validated with observed hourly pollutant concentrations obtained from an 18-mo residential air quality sampling program. Statistically, the model values of carbon monoxide are within 10% of the observed values in the concentration range interval which includes 85% of all hourly measurements; similarly, for nitric oxide the predicted values are within 15% of the observed; for nitrogen dioxide the difference between the predicted value and the ideal condition of exactly estimating the corresponding observed value is 16% for 85% of the observed hourly concentrations. Also, the GIOAP model predicts within 25% for nonmethane hydrocarbons and within 8% for carbon dioxide. Thus statistically the GIOAP model estimations are within 25% of the ideal condition (estimated and observed values coincide) for 85% of the observed values for CO, NO, NO_2, NMHC, and CO_2. The model has not been validated against sulfur dioxide owing to the very low values measured both indoors and outdoors. The predetermined validation criteria were not satisfied by the ozone model estimations; however, the calculated values were judged adequate because for about 85% of the observed values the predicted concentrations were within 2 ppb.

Sensitivity studies on the GIOAP model parameters indicate that errors in the estimation of the initial condition and the volume of the structure dissipate with time. Errors in estimating the air exchange rate, the indoor generation strength, and the indoor chemical decay rate are more significant. Sensitivity coefficients have been formulated for all input parameters.

The transient term is a unique feature of the GIOAP model; the impact of this term is substantial for stable pollutants but insignificant for ozone, which is a high reactive pollutant. The GIOAP Model, validated against a variety of measured data, satisfactorily predicts indoor pollutant concentrations, and it can be used to determine residential pollution levels under any conditions.

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SECTION 1

INTRODUCTION

Numerical simulation is considered among the most practical tools in estimating indoor air pollutant levels as a function of the outdoor pollutant levels plus other parameters. While its potential use has been realized by many scientists in the field, its application has been rather restricted, because the indoor-outdoor numerical models require inputs not readily available to the researcher. The extensive field program of the EPA-GEOMET project on the "Indoor Air Pollution Assessment Control and Health Effects" has provided a large data base. Using this information we have formulated the GEOMET Indoor-Outdoor Air Pollution (GIOAP) model.

The objective of the GIOAP model is to predict the indoor air pollution levels by simulating a series of complex interactions involving outdoor pollutant levels, structural characteristics of the examined dwellings, and behavioral patterns of the inhabitants.

The motivation for the formulation and application of the numerical model arises from the scientific recognition that measures to conserve energy within buildings, through the introduction of new energy transfer systems and the reduction of building ventilation rates, will result in changes in the indoor air quality characteristics. These changes may affect air quality either adversely or beneficially. Simulation of a large variety of indoor conditions will quantify these effects. In addition, the validated GIOAP model can be coordinated with an epidemiological study to determine the health effects of indoor air pollution.

The approach followed in the generation of the GIOAP model is a two-step procedure: (a) mathematical formulation, and (b) model validation. Each of these steps constitutes a section of this report and will be discussed in detail in the balance of this document.

The impact of a validated indoor-outdoor air pollution model will be substantial in identifying the optimum scenario that meets the national policy toward energy conservation measures in residential buildings without endangering the health of the segment of the population that spends a large portion of its time in the indoor residential environment. The last section of the document discusses the conclusions and impact of the GIOAP model.

SECTION 2

MATHEMATICAL FORMULATION

GENFRAL PRINCIPLES

The numerical simulation model formulated by GEOMET for assessing air quality in the indoor residential environment follows the general principles of a mass balance equation. In the sense that the GIOAP model specifically addresses residential environments (detached dwellings, row buildings, mobile homes, and apartments), it is different from the general models which include terms that are not applicable in the nonworkplace environment.

Air pollution in an enclosure may be of either outdoor or indoor origin, or both. If of outdoor origin, it enters through infiltration and ventilation. If of indoor origin, it is generated from pollutant sources within the enclosure. Regardless of source, air pollutants diffuse in the enclosure. They are removed over varying periods of time by exfiltration and ventilation to the outdoors and/or through indoor decay processes.

Air infiltration is defined as the change of air within a structure without the interference of the inhabitants. Thus the ambient air entering an enclosure through cracks in its walls is infiltrated air which, whether clean or contaminated, influences the indoor pollution levels. Ambient pollutants may also be introduced indoors through the ventilation process, which may be defined as air changes induced by the occupants of an enclosure; this can be natural ventilation through closing and opening of doors and windows, or can be forced ventilation through the operation of attic fans and air conditioning/heating systems. Air exfiltration is the opposite of air infiltration; indoor air leaves an enclosure through structural cracks. Exhaust ventilation moves air from indoors to outdoors through the vents of a forced circulation system as well as through door and window openings. Pollutants are introduced into the indoor environment by means of sources such as fireplaces, stoves, smoking, and cleaning devices. Finally, pollutants may be removed from the indoor air environment through indoor decay processes such as chemical transformation, settling, and absorption and adsorption by walls and furnishings (collectively termed pollutant sinks), and by filtering procedures in the makeup air or in the recirculated air.

To characterize time-dependent aspects of pollutant behavior, it is useful to deal with rates of change of air pollution within enclosures, rather than simply with absolute amounts of pollution. Mass balance principles require that the rate of change of an air pollutant quantity within an enclosure equals the sum of the rates of all pollutant introduction and removal processes that operate upon the enclosure.

THE GEOMET INDOOR-OUTDOOR AIR POLLUTION (GIOAP) MODEL

The GIOAP model illustrates the above general principles by specifically simulating procedures present in residential environments and is based upon the following mass balance equation:

$$V \frac{dC_{in}}{dt} = V\nu C_{out} + S - V\nu C_{in} - VDC_{in} \qquad (1)$$

where

C_{in} = the indoor pollutant concentration, mass/volume
C_{out} = the outdoor pollutant concentration, mass/volume
V = the volume of the building, volume
ν = the air exchange rate of the building, air exchange/time
S = the indoor source strength rate (rate of indoor pollutant emission), mass/time
D = the decay factor, time^{-1}.

The term on the left-hand of Equation (1) denotes the rate of change of the indoor pollutant mass. The first two terms on the right-hand side of the equation represent the rate by which the pollutant is introduced indoors, by infiltration of air ($V\nu C_{out}$) from outdoors, and by indoor pollutant generation due to indoor sources (S). The last two terms represent the pollutant removal rate due to exfiltration of indoor air ($V\nu C_{in}$), and due to indoor sinks, such as decay processes (VDC_{in}). The factor ν, the air exchange rate, appearing in the first and third terms of the right-hand side in Equation (1) is a total rate; it is the sum of the infiltration, exhaust, and ventilation rates.

A series of approximations are necessary before the GIOAP model can be applied to estimate the indoor air pollution levels. Over short time intervals simulated, the outdoor pollutant concentration is approximated by a straight line (an approach used by Shair and Heitner[1]). The line is given by:

$$C_{out} = m_{out}t + b_{out} \tag{2}$$

where m_{out} is the slope, t is the time, and b_{out} is the y-intercept. It is further assumed that the parameters ν, S, and D are constant during the time interval that is being modeled.

Thus the model equation becomes:

$$V \frac{dC_{in}}{dt} = V\nu(m_{out}t + b_{out}) - V\nu C_{in} + S - VDC_{in} \qquad t_0 \leq t \leq t_f$$

$$C_{in_0} \equiv C_{in}(t_0) \tag{3}$$

where C_{in_0} is the initial condition.

The estimations of the indoor pollutant concentrations are obtained from the solution to the initial value problem described by Equation (3). The closed-form solution to Equation (3) is given below:

$$C_{in}(t) = \left[C_{in_0} - m_{out}\left(\frac{\nu}{D+\nu}\right) t_0 - \left(\frac{1}{D+\nu}\right)\left(\nu b_{out} + \frac{S}{V} - \frac{m_{out}\nu}{D+\nu}\right)\right] e^{-(\nu+D)(t-t_0)}$$

$$+ \left(\frac{1}{D+\nu}\right)\left(\nu b_{out} + \frac{S}{V} - \frac{m_{out}\nu}{D+\nu}\right) + m_{out}\left(\frac{\nu}{D+\nu}\right) t \qquad t_0 \leq t \leq t_f \tag{4}$$

This is the equation used for numerical simulations of indoor air pollution levels.

The subject of relating the outdoor and indoor levels is relatively recent, and research emphasis has been placed on field measurements of contaminant levels rather than on the development of numerical models. Several scientists have attempted to formulate models employing relationships similar to the one expressed by Equation (3); Milly,[2] Calder,[3] Turk,[4] Hunt et al.,[5] Shair and Heitner,[1] and others have used more or less complex versions of Equation (3). The GIOAP model is specifically designed to simulate residential conditions. The assumptions concerning elements of the right-hand side of Equation (3) (S, ν, and D are constant over the time period being modeled, and C_{out} can be approximated by a straight line over the time period being modeled) are consistent with those made for other models. Previous studies have empahsized and simulated steady-state conditions; however, the GIOAP approach includes the transient portion of the solution to Equation (3). As a result, it is possible to model both short- and long-time intervals.

When Equation (4) is used in this study to model indoor air pollutant concentration levels, several additional assumptions are required. These assumptions are as follows:

1. The air exchange rate (ν) remains constant for at least 1 h.

2. The internal pollutant source rate (S) remains constant for at least 1 h.

3. The indoor pollutant removal procedure is modeled as a first-order decay term with the decay factor $D = \ln 2/t_{1/2}$, where $t_{1/2}$ is the half-life of the pollutant considered. For stable pollutants with long half-lives, D is approximated by zero. A list of the decay factors used in this study is given in Table 1.

The GIOAP model is capable of simulating any time interval, because the principles involved do not constrain this aspect. However, the time unit of the generally available ambient pollution data has led us to specify 1 h as the time resolution of the model. Finally, 1 h is the interval that is most appropriate for our purposes.

TABLE 1. DECAY FACTORS USED IN THE GEOMET INDOOR AIR POLLUTION STUDY

Pollutant	Decay factor (per hour)
CO	0.00
SO_2	1.04
NO	0.00
NO_2	1.39
O_3	34.66
CH_4	0.00
THC	0.00
CO_2	0.00
THC-CH_4	0.00

In order to model the indoor air pollutant behavior over the time interval $[t_0, t_f]$, the interval must be decomposed into the set of subintervals $(t_0, t_1]$, ... $(t_{n-1}, t_n]$ where $t_n = t_f$, and $t_i - t_{i-1} = 1$ h. As a result, Equation (3) becomes

$$C_i = \left[C_{i-1} - m_i\left(\frac{\nu_i}{D_i+\nu_i}\right) t_{i-1} - \left(\frac{1}{D_i+\nu_i}\right)\left(\nu_i b_i + \frac{S_i}{V} - \frac{m_i\nu_i}{D_i+\nu_i}\right)\right] e^{-(\nu_i+D_i)(t_i-t_{i-1})}$$

$$+ \left(\frac{1}{D_i+\nu_i}\right)\left(\nu_i b_i + \frac{S_i}{V} - \frac{m_i\nu_i}{D_i+\nu_i}\right) + m_i\left(\frac{\nu_i}{D_i+\nu_i}\right) t_i \qquad (5)$$

where

C_i = the indoor pollutant concentration level at time t_i, $i = 1, \ldots, n$

$C_{out}(t)$ = the outdoor pollutant concentration level at time t

$m_i = [C_{out}(t_i) - C_{out}(t_{i-1})]/(t_i - t_{i-1}), \; i = 1, \ldots, n$

$b_i = C_{out}(t_i) - m_i t_i, \; i = 1, \ldots, n$

S_i = internal source rate over the interval $(t_{i-1}, t_i]$, $i = 1, \ldots, n$

ν_i = air exchange rate over the interval $(t_{i-1}, t_i]$, $i = 1, \ldots, n$

V = volume of the building

D_i = decay factor over the interval $(t_{i-1}, t_i]$, $i = 1, \ldots, n$.

SECTION 3

MODEL VALIDATION

INTRODUCTION

The problem of estimating indoor air pollution levels involves both physical and behavioral parameters: the outdoor levels vary as a function of the local meteorology and other factors, while the indoor source strengths (indoor pollutant generation rates) and air exchange rates depend on the meteorology and the activity of the occupants. The combination of all inputs results in complex conditions that are rarely repeated or are very expensive to duplicate in the laboratory. Numerical models enable scientists to simulate these complex conditions, to stage specific incidents, and most importantly, to estimate values for the indoor pollutant concentrations.

Two essential stages determine the predictive capability of the GIOAP model:

1. Initial model validity. Do the predicted concentrations reflect observed data?

2. Model sensitivity. How do the predicted concentrations change in relation to changes in input parameter values?

An intrinsic element of these two stages is the ability to demonstrate the validity of the model using "best" estimates of the input model parameters. We have formulated a parameter estimation procedure that enables us to estimate the values of indoor source strengths and air exchange rates from the raw outdoor and indoor pollutant data. Recurring modes of pollution behavior, episodes, are of extreme importance in the Indoor Air Pollution EPA-GEOMET project. Numerically, a new episode is defined each time a new initial condition is introduced. It is our objective to associate each episode with stratified levels of indoor activity so that in the future we can estimate the indoor pollutant concentrations from outdoor pollution concentrations and indoor activity levels. The validity of these estimates will be studied in the balance of this section.

A three-step evaluation design will be followed in the assessment of the GIOAP model: we begin by estimating "best" values for input parameters, continue with statistical validation studies which include tables and input/output graphs, and conclude with a section on parameter sensitivity. This design takes advantage of the extensive data base available to this project.

PARAMETER ESTIMATION PROCEDURE

In order to estimate the indoor pollution levels using the GIOAP numerical model, all parameters associated with the model must be given numerical values. The monitoring data from the field studies of the indoor air pollution project constitutes a unique source of information for assigning numerical values to the relevant parameters. Some parameter values, such as initial indoor concentration and the volume of the structure, are easily determined; others, such as the air exchange rate (ν) of the building investigated and the internal pollutant generation source strength (S), are more difficult to obtain. The validity of the GIOAP model obviously depends on the values given to these difficult-to-quantify parameters. Since the model is to be validated under "best" conditions, we must obtain the best possible values for ν and S; the methodology used to obtain these values is the Parameter Estimation Procedure described in this section.

Theoretical Approach

Recall Equation (4):

$$C_{in}(t) = \left[C_{in_0} - m_{out}\left(\frac{\nu}{D+\nu}\right)t_0 - \left(\frac{1}{D+\nu}\right)\left(\nu b_{out} + \frac{S}{V} - \frac{m_{out}\nu}{D+\nu}\right)\right]e^{-(\nu+D)(t-t_0)}$$
$$+ \left(\frac{1}{D+\nu}\right)\left(\nu b_{out} + \frac{S}{V} - \frac{m_{out}\nu}{D+\nu}\right) + m_{out}\left(\frac{\nu}{D+\nu}\right)t \qquad t_0 \le t \le t_f \tag{4}$$

Also, consider the following function of S and ν:

$$f(S,\nu) = \sum_{i=1}^{n} [C_i(S,\nu) - CM_i]^2 \tag{6}$$

where

n = number of points
CM_i = i^{th} measured value; $i = 1, \ldots, n$
$C_i(S,\nu)$ = i^{th} computed value via Equation (4) corresponding to CM_i.

The fundamental problem in parameter estimation is to find value(s) of ν and S that minimize Equation (6). Two points must be made: (a) in the case of indoor air pollution studies, the parameters ν and S are constrained to lie within certain intervals specified by the nature of the investigated dwelling and the particular pollutant and source examined; and (b) Equation (4) is not linear in ν. These points combine to make the problem of estimating values for ν and S difficult.

A parameter estimation technique appropriate for the present problem is the grid search method. Although this process is easily constrained, it is lengthy, and its accuracy strongly depends on the number of grid points. Because $f(S,\nu)$ is a function of two variables, it is not possible to obtain the required minimum by the technique used for finding extreme values of functions of one variable that is taught to all students of beginning calculus. This technique is easily constrained over a given interval, but it cannot be applied to $f(S,\nu)$ because it minimizes only functions of one variable. However, the Parameter Estimation Procedure used in this study is a cross between the grid search and the optimization technique for a function of one variable. A sequence of five steps must be followed in the parameter estimation procedure.

1. Define the constraints on ν and S, i.e., $\nu_l \leq \nu \leq \nu_u$ and $S_l \leq S \leq S_u$, where subscripts l and u define the lower and upper values of the parameter intervals.

2. Determine $\Delta\nu = (\nu_u - \nu_l)/k$; where k is the number of intervals.

3. For a given $\nu_i = \nu_l + (i - 1)\,\Delta\nu$, $i = 1, \ldots, k + 1$, find the points S_{0_i} for which

$$\left.\frac{df(S,\nu)}{dS}\right|_{(S,\nu) = (S_{0_i},\nu_i)} = 0 \quad .$$

4. Determine S_{m_i} as the value of S that gives

$$\min\,\{f(S_l,\nu_i),\ f(S_{0_i},\nu_i),\ f(S_u,\nu_i)\} \quad .$$

5. The required estimates of ν and S are those values that give

$$\min\,\{f(S_{m_i},\nu_i) : i = 1, \ldots, k\} \quad .$$

The theoretical approach used in deriving this parameter estimation procedure is provided below. Owing to step 3 of the above sequence, all equations below refer to a given fixed value of the parameter ν. Equation (4) can be rewritten as follows:

$$C = \left[\frac{1 - e^{-(\nu+D)(t-t_0)}}{V(D+\nu)}\right] S$$
$$+ \left[C_0 - m\left(\frac{\nu}{D+\nu}\right) t_0 - \left(\frac{1}{D+\nu}\right)\left(\nu b - \frac{m\nu}{D+\nu}\right)\right] e^{-(\nu+D)(t-t_0)}$$
$$+ \left(\frac{1}{D+\nu}\right)\left(\nu b - \frac{m\nu}{D+\nu}\right) + m\left(\frac{\nu}{D+\nu}\right) t \qquad (7)$$

where

$C = C_{in}(t)$

$C_0 = C_{in_0}$

$m = m_{out}$

$b = b_{out}$

or as

$$C = \alpha S + \beta \tag{8}$$

where

$$\alpha = \frac{1 - e^{-(\nu+D)(t-t_0)}}{V(D+\nu)}$$

and

$$\beta = \left[C_0 - m\left(\frac{\nu}{D+\nu}\right) t_0 - \left(\frac{1}{D+\nu}\right)\left(\nu b - \frac{m\nu}{D+\nu}\right)\right] e^{-(\nu+D)(t-t_0)}$$

$$+ \left(\frac{1}{D+\nu}\right)\left(\nu b - \frac{m\nu}{D+\nu}\right) + m\left(\frac{\nu}{D+\nu}\right) t \quad .$$

From Equation (6) we have

$$f(S,\nu) = \sum_{i=1}^{n} (\alpha_i S + \beta_i - CM_i)^2 \tag{9}$$

where

α_i is computed @ $t = t_i$ and $t_0 = t_{i-1}$

β_i is computed @ $t = t_i$, $t_0 = t_{i-1}$, and $C_0 = CM_{i-1}$.

Equation (9) becomes

$$f(S,\nu) = S^2 \sum_{i=1}^{n} \alpha_i^2 + 2S \sum_{i=1}^{n} \alpha_i(\beta_i - CM_i) + \sum_{i=1}^{n} (\beta_i - CM_i)^2$$

$$f(S,\nu) = AS^2 + 2BS + C \tag{10}$$

where

$$A = \sum_{i=1}^{n} \alpha_i^2$$

$$B = \sum_{i=1}^{n} \alpha_i (\beta_i - CM_i)$$

$$C = \sum_{i=1}^{n} (\beta_i - CM_i)^2 \quad .$$

Equation (10) indicates that $f(S,\nu)$ is parabolic in S. The critical point is found by taking the derivative of f with respect to S:

$$\frac{df}{dS} = 2AS + 2B \quad . \tag{11}$$

Setting $df/dS = 0$, it is seen that $-(B/A)$ is a critical point; in order to determine whether $-(B/A)$ is a maximum or a minimum, the second derivative of f with respect to S is taken:

$$\frac{d^2f}{dS^2} = 2A \quad . \tag{12}$$

Since A is a sum of squares, $A > 0$, which means that

$$\left.\frac{d^2f}{dS^2}\right|_{S = -\frac{B}{A}} > 0$$

thus $S = -(B/A)$ minimizes $f(S,\nu)$.

Completion of the square in Equation (10) leads to the same conclusion:

$$f(S,\nu) = A\left(S + \frac{B}{A}\right)^2 + \left(C - \frac{B^2}{A}\right) \quad . \tag{13}$$

Again, since $A > 0$, the vertex $S = -(B/A)$ is the desired minimum.

The parameter S, representing the indoor pollutant generation rate, must be constrained to lie in a physically meaningful interval $[S_l, S_u]$. Thus, while $S = -(B/A)$ is an absolute minimum, $-(B/A)$ may not be within the interval $[S_l, S_u]$. Hence, in addition to computing $-(B/A)$, a test must be made to determine whether $-(B/A)$ lies in the interval (i.e., whether $-(B/A) \in [S_l, S_u]$); if not, the end points of the interval must be examined. The three cases to be considered are illustrated in Figure 1. They are:

Case 1: $S_{m_1} < S_l$

Case 2: $S_l \leq S_{m_2} \leq S_u$

Case 3: $S_u < S_{m_3}$.

In Case 1, the constrained minimum occurs at S_l; in Case 2, the constrained minimum occurs at S_{m_2}; and in Case 3, the constrained minimum occurs at S_u.

Application of the Parameter Estimation Procedure to the Indoor Air Pollution Data Base

In order to apply the Parameter Estimation Procedure to the Indoor Air Pollution Data Base, the problem of degrees of freedom must be considered; i.e., the fact that the number of observations used to estimate a set of parameters must be greater than the number of parameters being estimated. Thus as a means of increasing the amount of data available for use in the Parameter Estimation Procedure, the instantaneous outdoor values and instantaneous indoor averages for each 20-min segment of each hour were used because at this time the entire house is being modeled instead of individual zones.

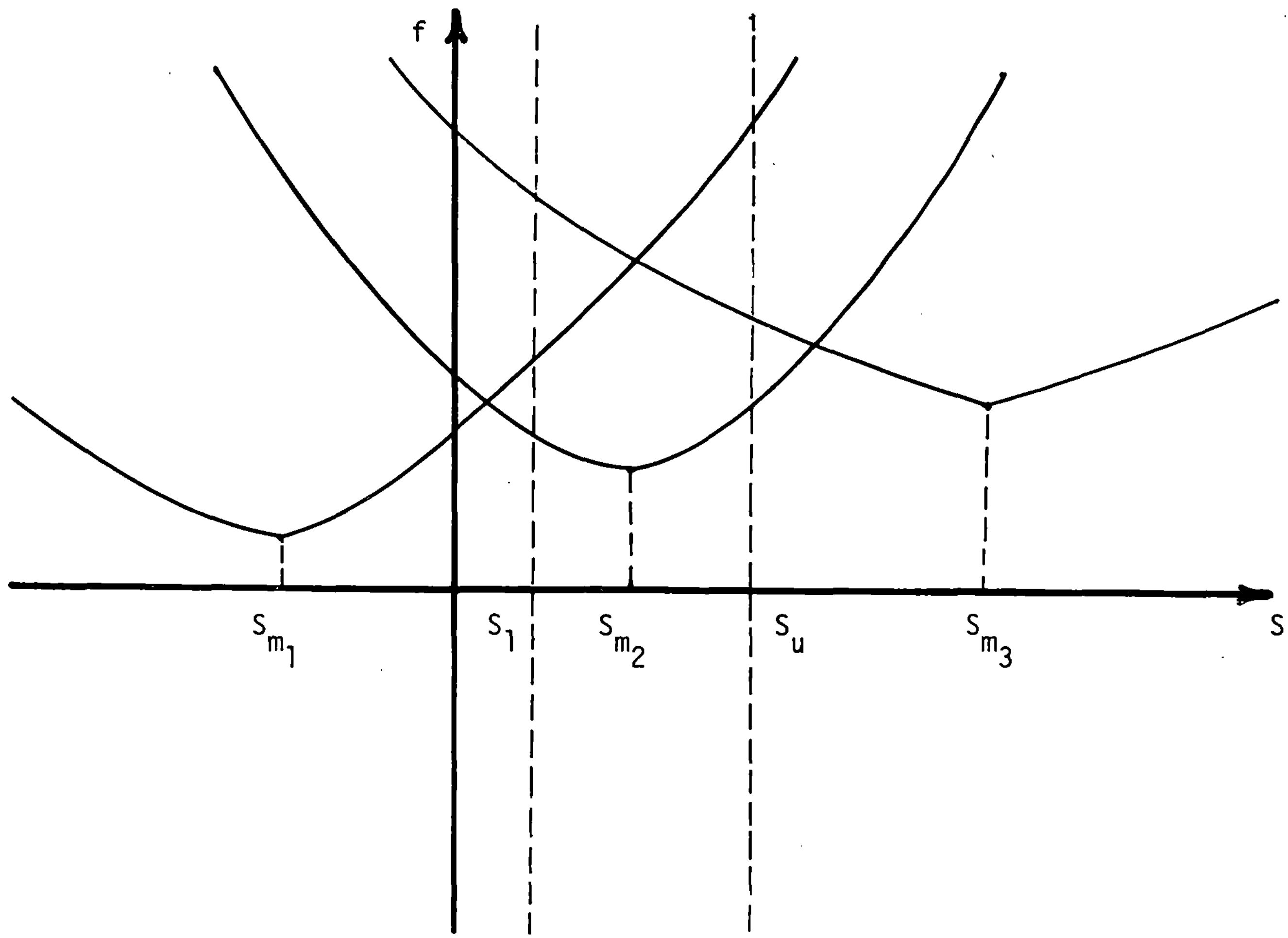

Figure 1. Graphical illustration for the three cases of constraints on interval source rate.

Hourly values of ν and S are desired; however, there is a problem in applying the Parameter Estimation Procedure to obtain hourly estimates of ν and S. The problem involves degrees of freedom. Even though three values are available for each hour to be used in the estimation, one of these is the initial value, which means that only two values can actually be used in the estimation procedure. As a result, the number of parameters to be estimated equals the number of points to be used, which means that no degrees of freedom are left for the estimation procedure.

The problem mentioned in the previous paragraph is resolved as follows: 2-h estimates of ν are calculated from the data of a "nonreactive pollutant," then, using these estimates of ν, hourly estimates of S are found for all pollutants. The "nonreactive" pollutant chosen was CO. If any of the 12 CO values (6 indoor and 6 outdoor over a 2-h period) are missing, ν is estimated using NO data; however, if both CO and NO data are missing for a given 2-h period, neither ν nor any of the pollutant source rates for that period is computed. Finally, if, for a given pollutant for a given hour, any values are missing, the corresponding source rate is not computed.

Essentially, we are using CO as a tracer to estimate theoretical values of air exchange rates for each of the investigated dwellings. As part of the field monitoring program of the Indoor Air Pollution project, the air exchange rate of each residence is determined experimentally. The tracer used for the experimental determination of the air exchange rate is sulfur hexafluroide (SF_6); the monitoring protocol calls for three or four different 4-h experiments per residence. The theoretical and experimental values for the air exchange rate agree in most of the investigated periods, and, in those cases of disagreement, the difference between the two values is not appreciable. Table 2 shows a comparison between the estimated and experimental values for the air exchange rates.

The estimated indoor source strength value S in mg/h is an "effective" pollutant production rate; i.e., the internal source is treated as if it operates for the entire 1-h period. The estimated indoor source is also comprehensive; that is, if two indoor sources are generating a pollutant simultaneously, the calculated theoretical value will be the sum of the individual source strengths. Using the daily logs kept by the occupants of the residences we monitored, we were often able to isolate a single source; the estimated theoretical values due to isolated indoor sources compare favorably with the available literature values.

TABLE 2. AIR EXCHANGE RATES

Residence	Air exchange rates: Estimated	Air exchange rates: Experimental
Chicago Experimental I	0.40 0 30 0.20	0.23 0.22 0.26
Pittsburgh Low-Rise Apt. I	0.64 0.58 0.60	0.60 0.84 0.63
Pittsburgh Mobile Home I	0.98 0.44	1.05 0.52
Denver Conventional	1.10	1.02
Washington Experimental I	0.10	0.60
Washington Conventional I	0.6 0.4 0.4	0.24 0.2 0.43
Baltimore Conventional I	1.2	0.78
Baltimore Experimental I	0.64	0.72

STATISTICAL STUDIES

The objective of the statistical studies performed on the GIOAP model is to define its ability to estimate indoor air pollution levels. In this document we evaluate the results from a sample of eight residences; this is a comprehensive review of the predictive power of the model.

In the first section we describe the procedure followed and outline the motivation and the objectives of each step. The section on the statistical assessment includes response graphs, statistical tables, and scatter diagrams.

In addition, it contains comments and conclusions on the model for each gaseous pollutant monitored. The final section provides theoretical details on sensitivity coefficients and includes a series of simulations that illustrate the errors introduced by not using the "best" estimated value for any given input parameter.

Statistical Procedure and Methodology

The strength of a theoretical or numerical method to predict air pollution levels has often been demonstrated with graphical illustrations. This has been the case in many studies with a small data base. Figures 2 and 3 present a sample of indoor values estimated by the GIOAP model against the observed indoor values for a number of pollutants during a 2-week monitoring period. While this randomly chosen set of illustrations indicates the predictive power of the model, it does not allow for general conclusions. In order to validate the GIOAP model a statistical approach is required.

A statistical analysis is performed on data sets consisting of pairs of hourly estimated and observed indoor air pollutant concentrations. A statistical approach is preferred to judgments made on the basis of comparing corresponding estimated and observed indoor air pollutant concentrations for two reasons. First, the GIOAP model simulates a variety of conditions for a number of pollutants and generates a large number of data sets, each of which contains many points (over 300). Second, direct comparison of estimated and observed values involves difficult judgments in deciding when the estimated value falls within an acceptable range of the observed value. Under such conditions statistical techniques provide fast, efficient, and reliable methods for assessing the data, thus making the judgments much less subjective.

The statistical analysis used to validate the GIOAP model is based on the principle that if the model simulates realistically the involved complex conditions, a plot of the estimated versus observed values would fall on or near a line with a slope of one and an intercept of zero.

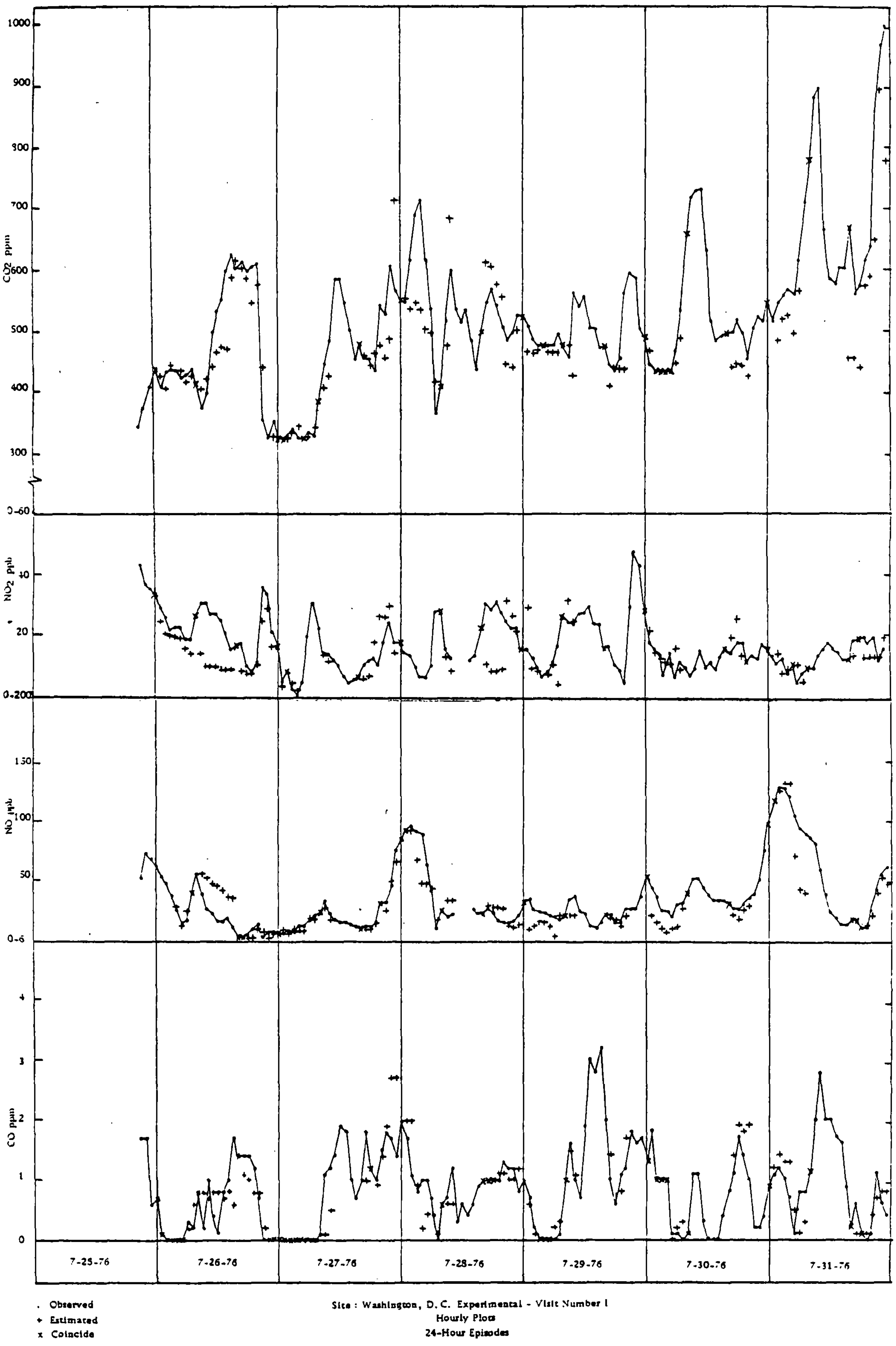

Figure 2. Estimated vs. observed pollutant concentrations for 7 consecutive days.

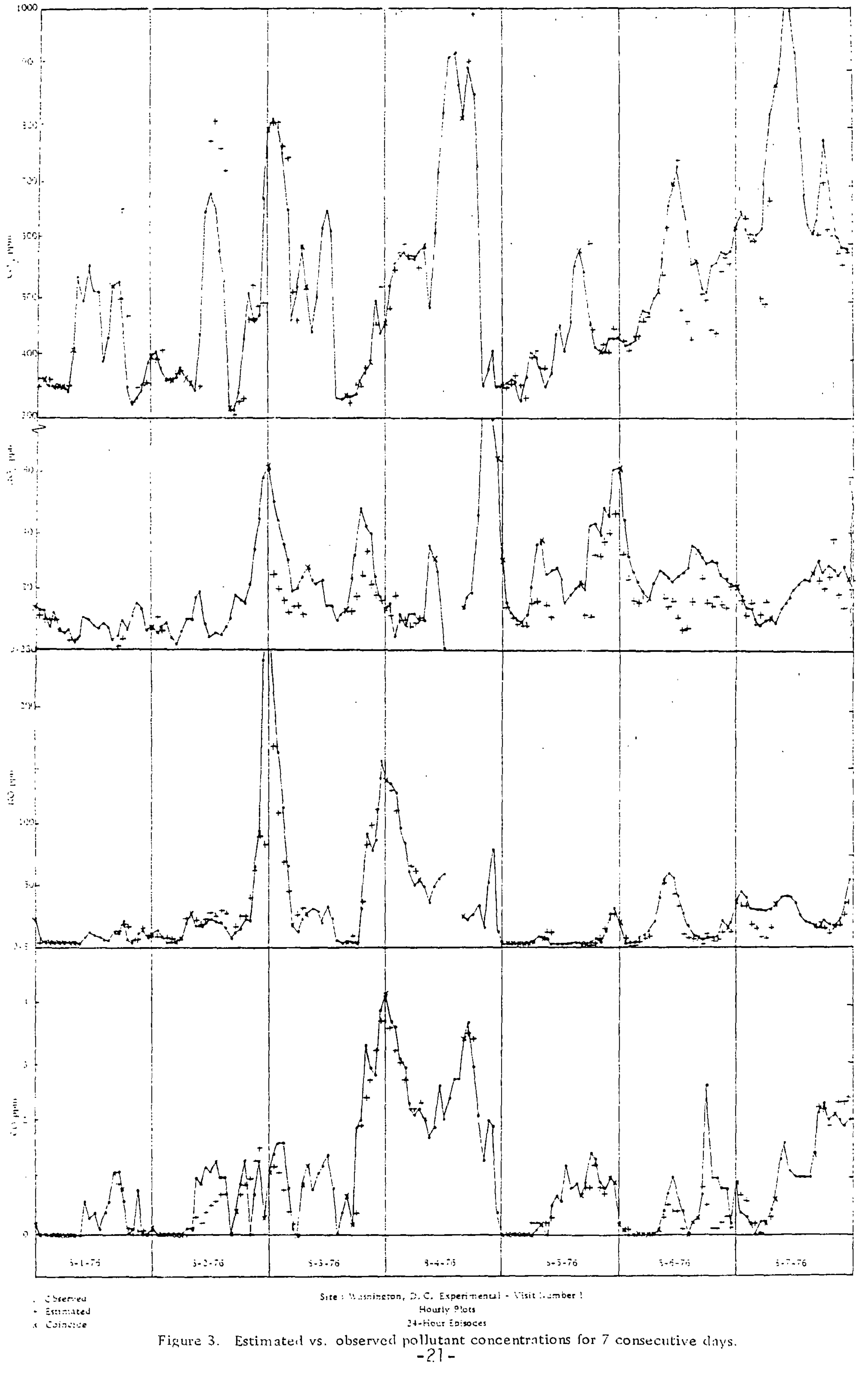

Figure 3. Estimated vs. observed pollutant concentrations for 7 consecutive days.

The problem of measuring the association between the observed and estimated values is divided in the following three sequential steps:

1. The degree of linearity in the relationship between the pairs of estimated and observed values is established. Linearity is required to proceed to step 2.

2. The slope and intercept of the line expressing the linear relationship between the observed and estimated values are determined. Criteria on the proximity of the slope and intercept to one and zero, respectively, are established and must be met before proceeding to step 3.

3. The degree of dispersion about the line defined by the slope and intercept in step 2 is calculated and must meet certain acceptability criteria.

The statistical methods used in each of the three steps will be discussed in the remainder of this subsection.

The Pearson product-moment correlation coefficient is calculated in order to determine whether or not a linear relationship exists between the pairs of estimated and observed values. The calculated correlation coefficient must be close to +1; if that is not the case, it should be concluded that the numerical model does not realistically simulate the processes involved.

The second step requires that the relationship be linear. A line is characterized by calculating the regression parameters (slope and intercept) of the plot of observed versus estimated values. In addition, the calculated slope and intercept values are tested for statistical significance. Each of the following hypotheses is statistically tested by a two-tailed t-test: (a) the slope is +1, and (b) the intercept is 0. In the following section it will become apparent that this statistical procedure will reject numerical estimations well within the accuracy limits of the input values. Thus, it is necessary to ease the limits that strict adherence requires by establishing a set of less restrictive criteria.

The final step is necessary only if a linear relationship exists between the estimated and observed values, and if the regression line meets the established criteria. This step determines how well the line fits the data points. In order to estimate the dispersion of the data points from the regression line, the Standard Error of Estimate (SEE) is calculated. If the SEE is small, the model data set is acceptable; if the SEE is large, it indicates that the points are widely scattered about the regression line and the modeled set should be rejected.

If a data set meets all these criteria, then it is concluded that the GIOAP model adequately represents the simulated event.

Statistical Assessment of the GIOAP Model

The statistical procedure outlined in the last section will be applied to eight sets of data corresponding to continuous monitoring from eight dwellings, each set consisting of seven gaseous pollutants. The model predicts the average indoor pollutant concentration for three different time periods (episodes), 3, 8, and 24 h. The model performance is evaluated for all days of the monitoring period.

The statistical information generated for each pollutant, each episode, and each residence is presented in tabular form (for example, see Table 3). The first column identifies the residence investigated, and the column labeled t_{epis} indicates the duration of each episode. The column labeled r contains the correlation coefficient; b is the intercept of the regression line corresponding to the plot observed versus estimated values, and m is the slope of this line. The null hypothesis--that the intercept is zero--is tested against the statistic t_b, while the null hypothesis--that the slope equals one--is tested against the statistic t_m. The column to the right of t_m contains the range of the average pollutant concentration observed indoors; this range provides a value against which the calculated standard error of estimate can be judged. The next to the last column presents the number of observations used for estimating the various statistics; it must be noted that this number is not always the total number of possible pairs because

TABLE 3. STATISTICAL DATA SUMMARY

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
	3-h									
	8-h									
	24-h									
	3 h									
	8-h									
	24-h									
	3-h									
	8-h									
	24-h									
	3-h									
	8 h									
	24-h									
	3-h									
	8-h									
	24-h									
	3-h									
	8-h									
	24-h									
	3-h									
	8-h									
	24-h									
	3-h									
	8-h									
	24-h									

of either missing observed values and/or missing calculated values due to the lack of the initial value, the air exchange rate, and/or the effective source strength.

Based on the information included in these columns, a conclusion is reached on how well the model predicts the indoor observed values. Three classes of acceptance or rejection comments are generated: Class I describes the simulations that satisfy all predetermined tests; Class II refers to numerical estimation of the indoor pollutant concentrations that, although not statistically acceptable, are judged to meet predetermined criteria which will be described below; and Class III refers to model estimations that do not meet any of the above requirements and must be rejected because they do not realistically simulate the observed indoor values.

The investigation of the model performance for each pollutant will be presented in the balance of this section. It is however essential to begin by stating a set of rules for each of the classes outlined in the previous paragraph. Since there are varying degrees of linearity, a decision must be made on the cutoff level of the correlation coefficient. Figures 4 through 7 are scatter diagrams with four different correlation coefficients; their values are $r = 0.96$, $r = 0.82$, $r = 0.72$, and $r = 0.66$, respectively. The cutoff value chosen for this study for the correlation coefficient is $r = 0.7$; thus if r is below 0.7 the relationship between the observed and estimated value is considered nonlinear for the purposes of this study.

For Class I acceptance the criteria on b and m are set by the two-tailed statistical t-test. For a significance level of 0.01 the t value $t_{0.005,\infty} = 2.576$ (the number of degrees of freedom is considered to be infinite because in this project it is almost always larger than the maximum finite degrees of freedom specified in the statistical tables); thus if either t_b or t_m is outside the interval $-2.576 \leq t \leq 2.576$, the estimated indoor pollutant concentrations do not fall into Class I.

For Class II, predetermined acceptability limits can be placed on the slope m for all pollutants. However, limits on the intercept must be determined on a case basis since the proximity to zero of the intercept

MODEL VALIDATION - 8-H CO 08/12/77 PAGE 2

FILE P6135 (CREATION DATE = 08/12/77) INDOOR AIR POLLUTION MODEL VALIDATION
SCATTERGRAM OF (DOWN) OBS OBSERVED POLLUTANT CONCENTRATION (ACROSS) EST ESTIMATED POLLUTANT CONCENTRATIO

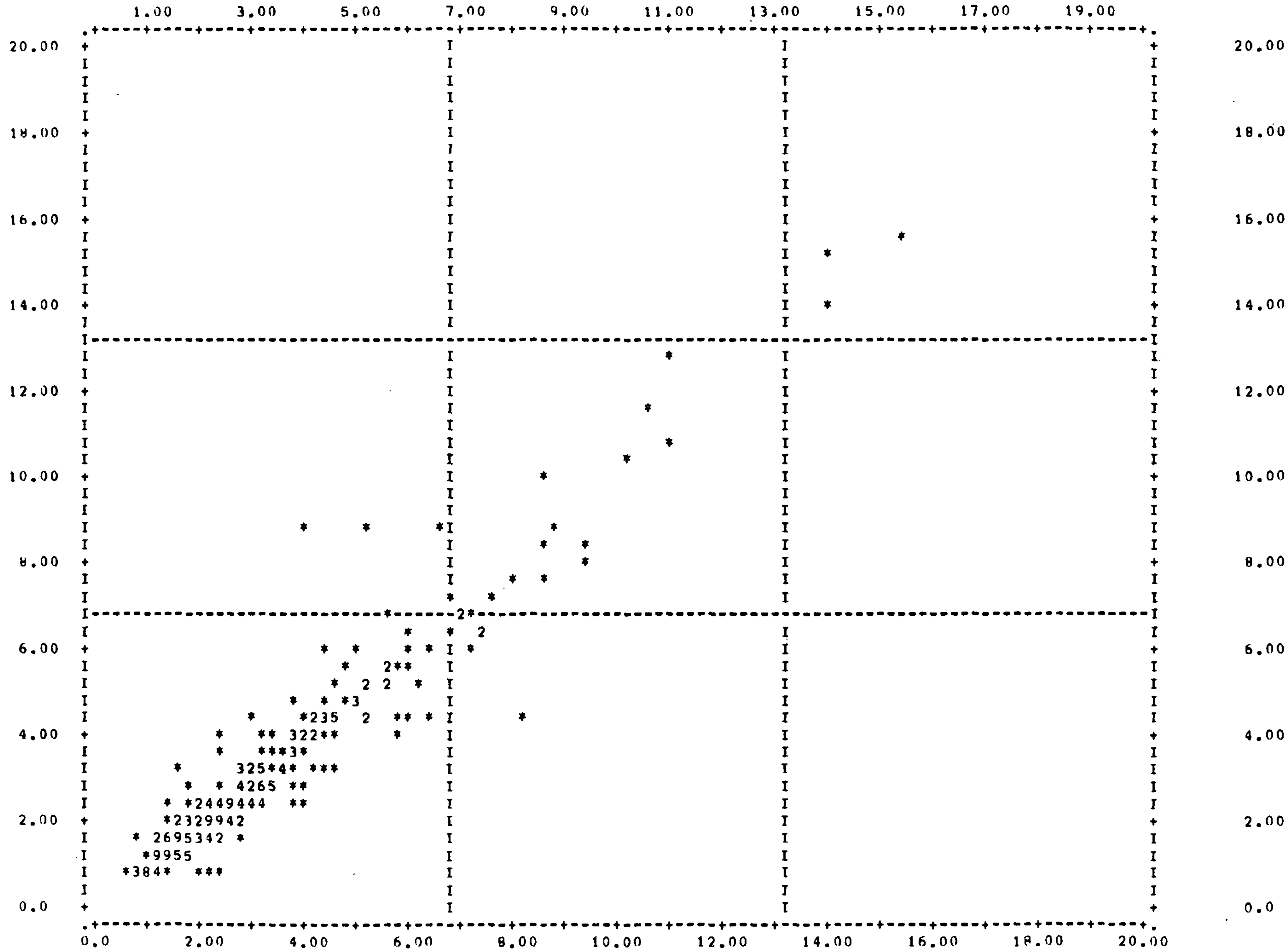

Figure 4. Scatter diagram with r = 0.96.

MODEL VALIDATION - WASHINGTON CONVENTIONAL 1 8-H NO2 02/08/78 PAGE 2

FILE P6135 (CREATION DATE = 02/08/78) INDOOR AIR POLLUTION MODEL VALIDATION
SCATTERGRAM OF (DOWN) OBS OBSERVED POLLUTANT CONCENTRATION (ACROSS) EST ESTIMATED POLLUTANT CONCENTRATIO

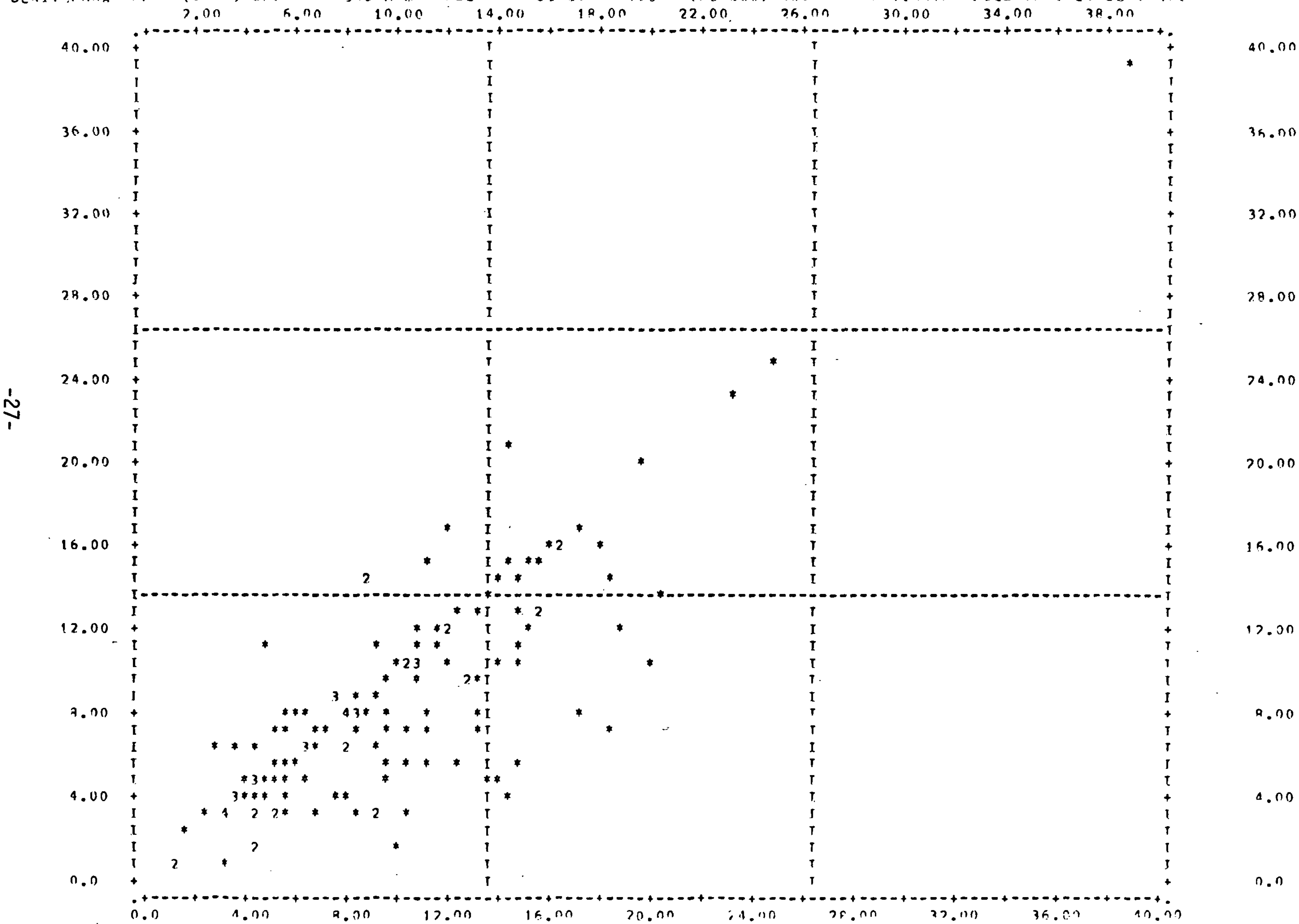

Figure 5. Scatter diagram with r = 0.82.

MODEL VALIDATION 24-H THC-CH4 08/16/77 PAGE 2

FILE P6135 (CREATION DATE = 08/16/77) INDOOR AIR POLLUTION MODEL VALIDATION
SCATTERGRAM OF (DOWN) OBS OBSERVED POLLUTANT CONCENTRATION (ACROSS) EST ESTIMATED POLLUTANT CONCENTRATIO

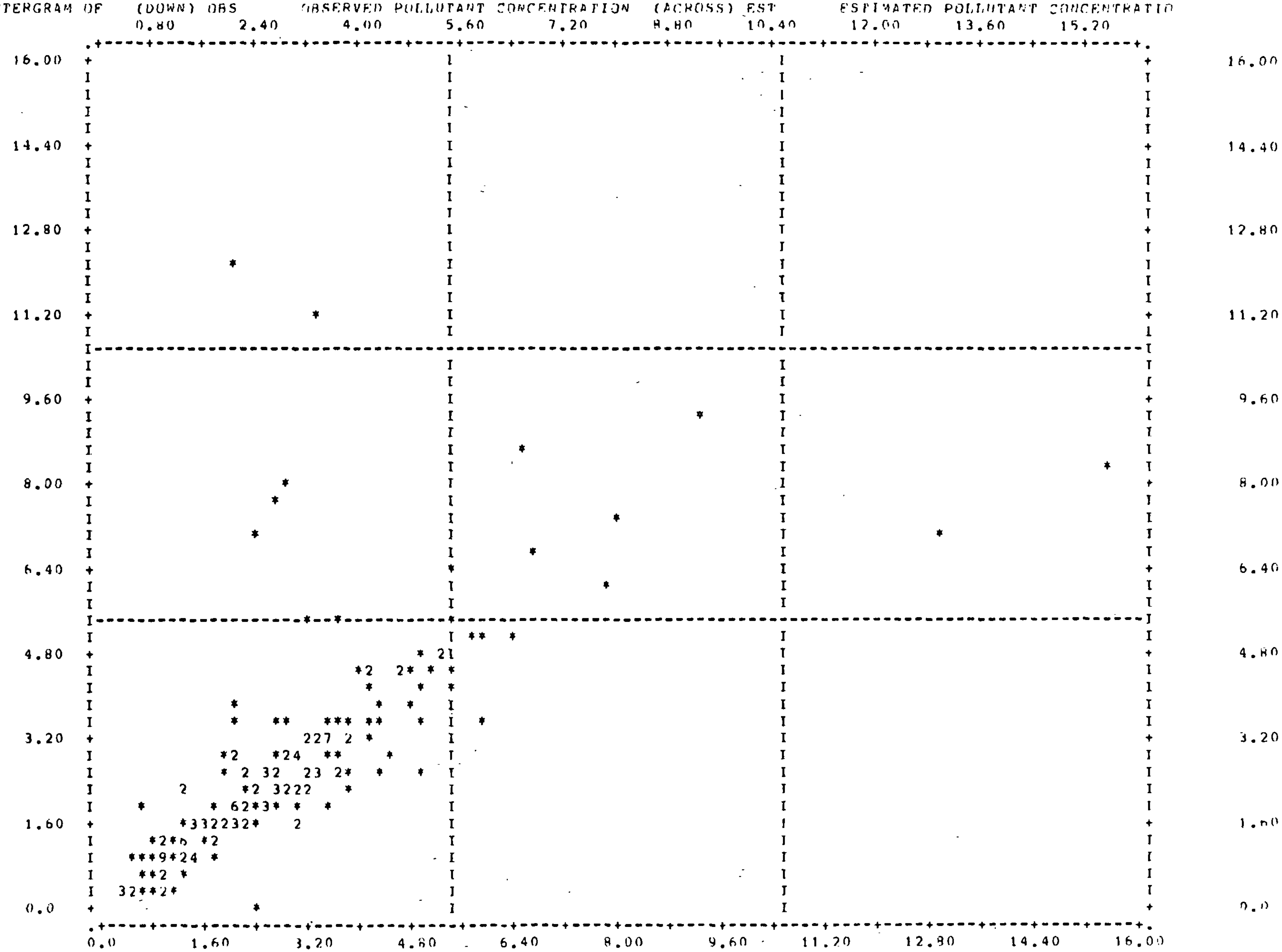

Figure 6. Scatter diagram with r = 0.72.

MODEL VALIDATION - DENVER CONVENTIONAL P-H SO2   02/08/78   PAGE 2

FILE P6135 (CREATION DATE = 02/08/78) INDOOR AIR POLLUTION MODEL VALIDATION
SCATTERGRAM OF (DOWN) OBS OBSERVED POLLUTANT CONCENTRATION (ACROSS) EST ESTIMATED POLLUTANT CONCENTRATIO

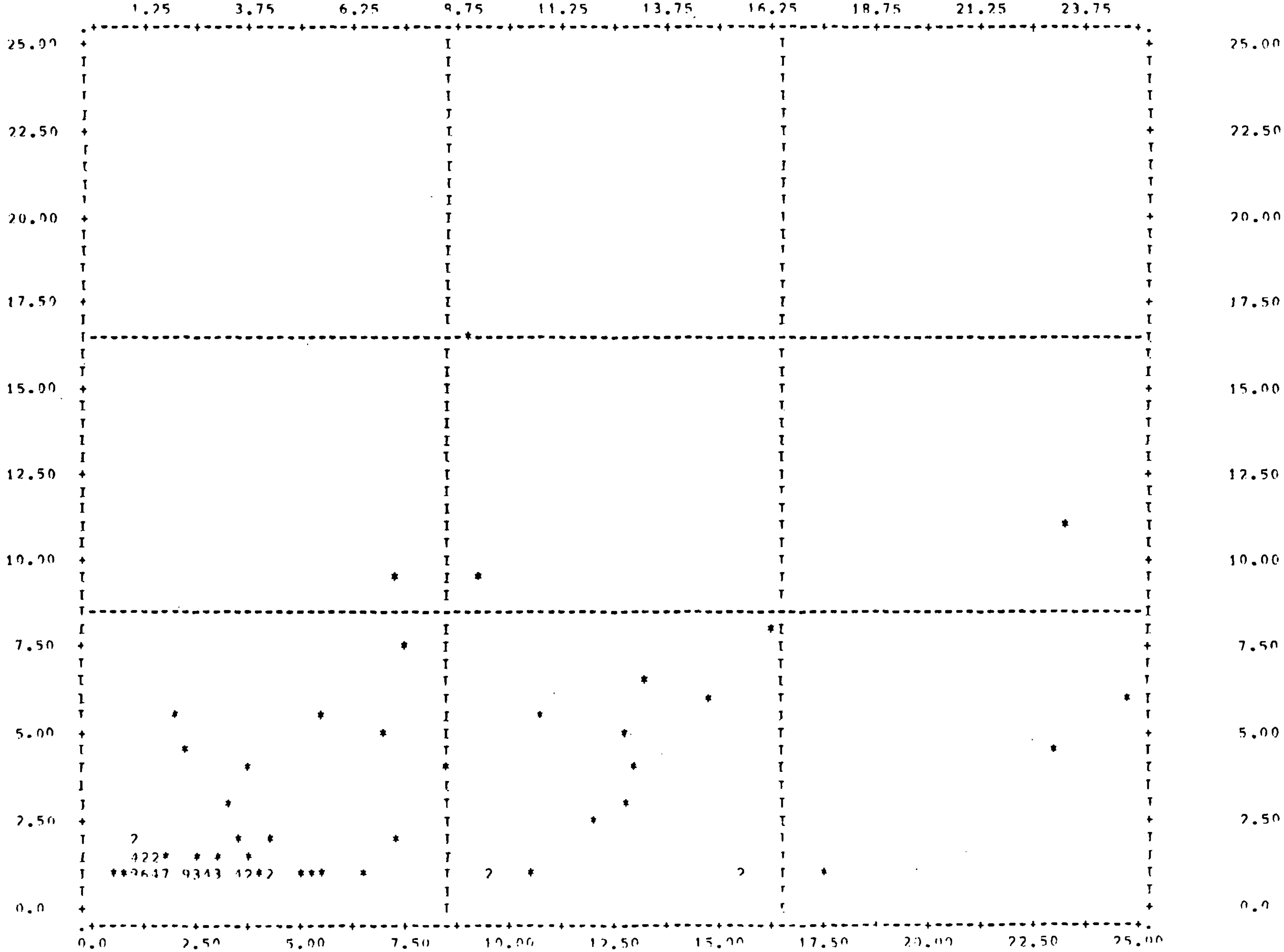

Figure 7. Scatter diagram with r = 0.62.

crucially depends on the range of the observed values which varies from pollutant to pollutant. In Class II, slope values within the closed interval [0.7, 1.3] are acceptable. In addition, values of the intercept that have magnitude greater than 15% of the maximum observed pollutant concentration are rejected. The last criterion for acceptance in Class II requires that the Standard Error of Estimate (SEE) is $\leq$ 10% of the maximum observed value.

When examining the tables containing the statistical validation data for each pollutant (i.e., Tables 4 through 7 and 10 through 12), it will be seen that the following phenomenon occurs several times: for a given set of conditions the 3- and/or 8-h episodes will be Class II, but the corresponding 24-h episode will be Class I. Further examination will reveal that the 24-h episode statistical data is based on fewer observations than either the 3- or 8-h episode data. The reason for this is that, when missing data are encountered, the model calculations cease regardless of whether the end of the episode has been reached. Thus, some episodes span fewer hours than are indicated by the headings, a condition which results in less overall variation and gives better statistical data.

In the balance of this section each pollutant will be examined individually.

Carbon Monoxide--

Table 4 provides all the statistical information obtained by the previously outlined steps for CO. In all cases investigated an acceptable degree of linearity exists ($r \geq 0.821$), the intercept is uniformly close to zero, and the slope is outside the prescribed interval only once ($m = 1.336$ for the 24-h episode in the Pittsburgh Low-Rise Apt. I); this is the only Class III case simulated. Let us investigate this Class III case in more detail. The following points can be made:

1. Frequency distribution tables show that 91% of the sampled values fall in the half-open interval [0, 2.8).

TABLE 4. STATISTICAL DATA SUMMARY FOR CARBON MONOXIDE (CO ppm)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.943	0.174	0.911	4.779	-5.039	0.0-6.2	0.310	337	II
	8-h	0.900	0.242	0.874	4.810	-5.096		0.389	293	II
	24-h	0.912	0.173	0.919	3.119	-2.553		0.268	174	II
Denver Conventional	3 h	0.970	0.041	0.980	0.744	-1.471	0.89-15.9	0.570	320	I
	8-h	0.959	0.018	1.006	0.259	0.333		0.683	291	I
	24-h	0.949	-0.024	0.993	-0.286	-0.285		0.549	168	I
Chicago Experimental I	3-h	0.947	0.289	0.943	5.768	-3.004	0.33-6.33	0.352	282	II
	8-h	0.888	0.683	0.862	9.350	-4.616		0.520	224	II
	24-h	0.920	0.70	0.796	9.293	-6.890		0.462	133	II
Pittsburgh Low-Rise Apt. I	3-h	0.884	-0.029	1.128	-5.90	3.40	0.0-7.0	0.519	253	II
	8 h	0.821	0.023	1.218	0.348	3.778		0.652	217	II
	24-h	0.878	-0.105	1.336	-1.378	5.143		0.571	126	III
Baltimore Experimental I	3-h	0.967	0.001	1.005	0.264	0.308	0.0-2.0	0.077	235	I
	8-h	0.969	0.004	1.096	0.709	5.062		0.075	213	II
	24-h	0.960	-0.003	1.034	0.525	1.419		0.067	162	I
Washington Conventional I	3-h	0.961	0.040	0.972	1.222	-1.913	0.0-5.2	0.396	360	I
	8-h	0.938	-0.003	0.949	-0.068	-2.543		0.487	305	I
	24-h	0.912	0.019	1.004	0.390	0.130		0.475	200	I
Baltimore Conventional I	3-h	0.851	0.107	0.778	3.683	-8.038	0.0-4.56	0.389	305	II
	8-h	0.876	0.036	0.882	1.178	-3.734		0.349	240	II
	24-h	0.916	0.034	0.894	1.235	-3.363		0.271	154	II
Washington Experimental I	3-h	0.930	0.080	0.942	3.224	-2.740	0.0-4.22	0.314	313	II
	8-h	0.889	0.117	0.883	3.594	-4.175		0.391	265	II
	24-h	0.895	0.087	0.948	2.50	-1.427		0.358	169	II

2. Straightforward calculations using the following relationship

   Observed Value = Intercept + (Slope) (Estimated Value)

   indicate that the approximate maximum difference between observed and estimated values is 22% of the observed value.

A similar analysis applied to a randomly chosen Class II case gives an approximate maximum difference between observed and estimated values of 2% of the observed CO value. Analyses of this nature for a Class I case provide similar or better results. It is concluded that the model predicts CO indoor values acceptably.

Nitric Oxide--

Table 5 illustrates a strong linear correlation between observed and estimated values, $r \geq 0.875$. Similarly, the slopes of the calculated regression lines lie within the predetermined interval. As a first observation, the magnitude estimated for the intercept and the standard estimates of error may seem large; however, when compared with the indicated ranges of the monitored values, they are put in proper perspective and are judged acceptable. Thus, 21 cases are accepted as Class II, while the remaining 3 cases are accepted as Class I.

In order to provide a perspective on the model performance, an approximate estimate of the percent difference between observed and estimated values will be calculated. The Denver Conventional Residence is chosen because it was one of the extreme cases considered. Let us investigate the 8-h episode simulations. The relevant statistics are $r = 0.875$, $b = 10.135$, and $m = 0.793$. Frequency distributions of observed indoor averages generated for the data interpretation task of this study show that 94% of the hourly values fall within the half-open interval [0, 120). Following the thinking expressed for CO, we conclude that for this case, within the specified interval, the approximate maximum difference between observed and estimated values is 15% of the observed value; or within this interval the statistical model value is at most 1.15 times the observed value.

TABLE 5. STATISTICAL DATA SUMMARY FOR NITRIC OXIDE (NO ppb)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.970	6.873	0.962	2.377	-2.912	77-467	22.295	335	II
	8-h	0.941	5.192	0.990	1.159	-0.480		29.690	274	I
	24-h	0.917	12.541	0.931	2.213	-2.366		29.452	193	I
Denver Conventional	3 h	0.909	8.307	0.798	4.304	-9.899	2.1-409	25.288	323	II
	8-h	0.875	10.135	0.793	4.072	-8.203		31.605	305	II
	24-h	0.911	1.236	0.912	0.543	-2.550		18.175	147	I
Chicago Experimental I	3-h	0.987	1.907	0.941	3.531	-6.753	0.0-256	6.513	320	II
	8-h	0.970	3.479	0.913	3.720	-6.003		10.281	251	II
	24-h	0.976	4.733	0.836	4.642	-10.686		8.947	151	II
Pittsburgh Low-Rise Apt. I	3-h	0.982	-1.135	1.034	-2.03	3.014	4.11-300.1	7.233	316	II
	8 h	0.982	-2.355	1.066	-3.525	5.101		7.805	258	II
	24-h	0.993	-2.235	1.048	-3.603	4.775		5.717	155	II
Baltimore Experimental I	3-h	0.939	1.231	1.026	3.656	1.202	0.0-87.2	5.334	300	II
	8-h	0.948	1.740	1.042	5.270	1.958		4.983	221	II
	24-h	0.946	2.402	1.039	6.239	1.596		5.327	221	II
Washington Conventional I	3-h	0.986	5.542	0.975	5.325	-2.619	18.6-279	9.101	303	II
	8-h	0.966	15.105	0.919	7.784	-4.711		14.303	210	II
	24-h	0.953	25.878	0.809	8.988	-7.957		15.482	117	II
Baltimore Conventional I	3-h	0.906	2.314	0.841	2.328	-7.159	1.0-224.1	14.139	316	II
	8-h	0.954	0.706	0.927	0.960	-3.969		9.235	252	II
	24-h	0.961	0.207	0.931	0.256	-3.421		8.657	177	II
Washington Experimental I	3-h	0.935	1.120	1.058	1.085	2.527	0.0-283.8	13.320	312	II
	8-h	0.918	2.052	1.052	1.560	1.829		15.818	263	II
	24-h	0.906	1.841	1.066	0.924	1.721		19.272	169	II

This specific analysis is of course an example; however, we think that the model realistically simulates indoor average concentration for nitric oxide.

Nitrogen Dioxide--

Numerical simulations of indoor NO_2 concentrations require the use of a first-order decay term. The half-life used for these simulations is 30 min; this value is suggested by observations of the indoor instantaneous NO_2 values of this project as well as by Wade et al.[6] and by Craig Hollowell in a private communication. The use of first-order chemical decay terms, instead of the zero order rate used originally, has substantially improved the predictive power of the model. Six cases are rejected, 3 cases are accepted as Class I, and 15 cases are accepted as Class II. The cases that have been rejected are in residences without indoor NO_2 sources; the indoor concentrations are persistently low with very little variation. In cases like this the model may overestimate the indoor NO_2 concentrations by as much as 50%. However, the model performs well for a total of 18 cases (out of 25); see Table 6. The maximum difference between the statistical model value and the observed value is 16%. This conclusion is reached by the process described for CO, and it refers to a specific example; however, the general assessment is that the GIOAP is realistically simulating indoor average concentrations for NO_2.

Sulfur Dioxide--

The nature of the SO_2 data is a source of the apparent inability of the model to estimate the observed indoor values (see Table 7). Table 8 shows portions of the indoor average concentration frequency distribution for SO_2. Note that the instrument used, a Meloy OA-185-2A commercial detector, has a limit of detection of 13.1 $\mu g/m^3$ (0.005 ppm). It is apparent that almost all SO_2 values observed indoors are at or below the instrument's lower limit of detection.

Three factors influence these low levels of SO_2: (a) the observed SO_2 outdoor levels are generally low; (b) the pollutant is a moderately reactive gas; therefore, the indoor levels are lower than the outdoor levels; and

TABLE 6. STATISTICAL DATA SUMMARY FOR NITROGEN DIOXIDE (NO_2 ppb)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.834	1.093	0.838	1.961	-5.326	0.0-75.3	5.770	334	II
	8-h	0.773	1.265	0.832	1.712	-4.045		6.616	272	II
	24-h	0.708	2.630	0.718	2.943	-5.451		6.662	193	II
Denver Conventional	3 h	0.875	8.045	0.803	6.696	-7.919	11-138	8.604	321	II
	8-h	0.744	12.349	0.711	7.249	-7.773		11.256	298	II
	24-h	0.835	6.012	0.837	3.371	-3.429		5.578	137	II
Chicago Experimental I	3-h	0.651	6.106	0.725	13.324	-5.757	0.0-39.3	5.058	316	III
	8-h	0.487	7.558	0.677	13.148	-4.196		6.072	251	III
	24-h	0.475	7.684	0.868	9.623	-0.999		6.779	151	III
Pittsburgh Low-Rise Apt. I	3-h	0.918	-0.400	0.946	-1.635	-2.312	0.0-31.1	2.646	315	I
	8 h	0.871	-0.317	0.873	-0.938	-4.142		3.222	257	II
	24-h	0.839	-0.255	0.837	-0.606	-3.732		3.103	155	II
Baltimore Experimental I	3-h	0.750	2.779	0.661	8.549	-9.963	0.0-41.1	3.755	295	III
	8-h	0.679	3.448	0.571	10.035	-11.074		3.937	255	III
	24-h	0.570	4.176	0.492	10.850	-10.229		3.915	206	III
Washington Conventional I	3-h	0.847	0.192	0.925	0.469	-2.051	0.0-38.8	3.113	253	I
	8-h	0.823	0.567	0.809	1.085	-4.090		3.005	144	II
	24-h	0.773	0.856	0.739	1.086	-3.223		2.424	58	II
Baltimore Conventional I	3-h	0.758	7.398	0.707	7.099	-8.452	1-130.6	10.039	309	II
	8-h	0.836	5.574	0.764	6.075	-7.224		7.085	237	II
	24-h	0.925	1.879	0.934	2.458	-2.269		4.988	177	I
Washington Experimental I	3-h	0.854	3.492	0.968	4.902	-0.934	0.0-95.2	6.637	296	II
	8-h	0.728	5.981	0.888	5.583	-1.984		7.756	224	II
	24-h	0.758	4.372	0.939	3.594	-0.861		7.246	131	II

TABLE 7. STATISTICAL DATA SUMMARY FOR SULFUR DIOXIDE (SO_2 ppb)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.491	4.848	0.142	16.172	-60.011	3.0-29.1	4.028	314	III
	8-h	0.488	4.346	0.130	12.044	-59.732		4.262	258	III
	24-h	0.517	3.963	0.152	7.916	-44.596		4.682	176	III
Denver Conventional	3 h	0.692	0.725	0.361	8.575	-30.321	1.0-16	1.262	321	III
	8-h	0.619	0.778	0.277	9.021	-35.481		1.253	300	III
	24-h	0.713	0.696	0.259	7.091	-37.442		1.055	168	III
Chicago Experimental I	3-h	0.603	1.342	0.489	9.946	-14.083	2-19.8	1.089	320	III
	8-h	0.464	1.789	0.341	11.292	-15.973		1.214	252	III
	24-h	0.574	1.350	0.449	7.235	-10.652		1.012	155	III
Pittsburgh Low-Rise Apt. I	3-h	0.511	0.414	0.226	4.002	-35.463	0.0-110	1.463	304	III
	8 h	0.505	0.398	0.166	3.417	-45.249		1.455	240	III
	24-h	0.514	0.488	0.159	3.246	-40.140		1.548	164	III
Baltimore Experimental I	3-h	0.0	2.0	0.0	0.0	0.0	2.0-4.2	0.0	299	III
	8-h	0.948	1.740	1.042	5.270	1.958		4.983	269	III
	24-h	0.946	2.40	1.039	6.239	1.596		5.327	221	III
Washington Conventional I	3-h	0.945	-0.169	1.113	-1.705	5.506	3-9.7	0.744	357	II
	8-h	0.919	-0.474	1.231	-3.487	7.582		0.874	301	II
	24-h	0.906	-0.800	1.326	-4.366	7.413		0.896	200	III
Baltimore Conventional I	3-h	0.704	1.127	0.448	15.164	-20.740	1.8-114	0.668	290	III
	8-h	0.627	1.384	0.329	15.933	-24.627		0.809	228	III
	24-h	0.825	1.006	0.472	11.709	-20.109		0.630	154	III
Washington Experimental I	3-h	0.140	1.920	0.041	57.273	-58.279	1.4-2.5	0.063	313	III
	8-h	0.051	1.985	0.008	92.926	-96.717		0.060	264	III
	24-h	0.050	1.993	0.007	89.566	-95.012		0.061	168	III

(c) the flame photometric principle of detection, employed in the commercial instrument used in the field operations, is subject to negative interference from CO_2. The instrument, although "approved" by EPA for sampling in the outdoor ambient environment, is subject to quenching by CO_2, which is present in high levels in the indoor environment. The extent of the negative CO_2 interference on the SO_2 levels is illustrated in Table 9, which shows the results of four tests performed by the field team of this project. In each case the same correction factor is calculated; however, we have not undertaken such corrections because the observed levels are almost always close to very low, unreliable levels.

TABLE 8. SO_2 FREQUENCY DISTRIBUTION

Residence	Percentage	SO_2 Range in ppb
Pittsburgh Mobile Home I	44.2	3.00 - 5.60
	35.2	5.60 - 8.20
Denver Conventional	90.5	1.00 - 2.50
Chicago Experimental I	80.0	2.00 - 3.80
	15.6	3.80 - 5.60
Pittsburgh Low-Rise Apt. I	60.9	0.00 - 1.00
	20.7	1.00 - 2.00
Baltimore Experimental I	99.7	2.00 - 2.20
Washington Conventional I	60.5	3.70 - 4.40
	28.8	7.90 - 8.60
Baltimore Conventional I	94.9	2.00 - 2.90
Washington Experimental I	98.8	2.00 - 2.12

TABLE 9. NEGATIVE CO_2 INTERFERENCE ON SO_2 LEVELS*

Test No.	$[CO_2]$ Introduced into the SO_2 Monitor	$[SO_2]$ Output by the Instrument	$[SO_2]$ Introduced into the Instrument
1	300	0 33	0. 33
	813	0. 265	0. 33
	1460	0. 205	0. 33
	1975	0. 165	0. 33
2	300	0. 23	0. 23
	833	0. 18	0. 23
	1450	0. 14	0. 23
	1975	0. 115	0. 23
3	308	0. 095	0. 095
	850	0. 075	0. 095
	1500	0. 055	0. 095
	2037	0. 045	0. 095
4	312	0. 050	0. 050
	872	0. 040	0 050
	1525	0. 030	0. 050
	2088	0. 023	0. 050

* All concentration levels in ppm.

The point here is that while the model does not simulate the observed SO_2 concentrations, both the estimated values and the observed values are too low and too close to zero to justify employment of correction factors. It is concluded that the model's ability to correctly estimate SO_2 values has not been tested by the available data. SO_2 levels have been found to be low in the indoor environment not only by the present study but in all similar studies. Sulfur dioxide concentrations decay at rates similar to NO_2; thus it is expected that the GIOAP model would realistically simulate higher and more variable indoor levels.

Ozone--

An ozone table similar to the statistical summary tables for the other pollutants would indicate that the model does not satisfy the predetermined criteria. However, it is misleading to consider the model performance as unsatisfactory because the majority of the estimated values are within 3.92 $\mu g/m^3$ (2 ppb) of the observed values; this difference is smaller than the monitor's precision. The observed ozone levels in the indoor environment are low and often constant for long periods. The small variations in the predicted values weigh heavily in the estimation of correlation coefficients and other statistics that assess the power of the model to predict. The capability of the GIOAP model to predict indoor ozone levels is judged adequate because it gives a realistic picture of the ozone variation indoors. Finally, the linear dynamic model(1) has been utilized to predict higher indoor levels, and its use in conjunction with the GIOAP model is recommended.

Nonmethane Hydrocarbons--

The model simulates the majority of the investigated cases well. The model requires knowledge of the molecular weight of the pollutant examined; in the case of hydrocarbons we had to use an average molecular weight representing the hydrocarbons most often sampled. Thus the uncertainty introduced may have caused some of the Class III judgments. In spite of this uncertainty, Table 10 indicates that the GIOAP model estimates the indoor nonmethane hydrocarbon levels satisfactorily in the majority of the cases examined.

Methane--

Table 11 illustrates that the model estimates the indoor methane values realistically. As always, 24 cases are run. For this pollutant, 2 are judged Class III, 17 are accepted as Class II, and 5 are classified as Class I. Following the techniques used in previous pollutant analysis, we estimate a maximum difference of approximately 30% between the statistically estimated CH_4 concentration and its corresponding observed value. This is one of the largest percent differences found in Table 11.

TABLE 10. STATISTICAL DATA SUMMARY FOR NONMETHANE HYDROCARBONS (THC-CH_4 ppm)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.819	1.036	0.585	10.996	-18.596	0.0-13	1.189	338	III
	8-h	0.745	0.884	0.665	6.752	- 9.451		1.365	285	III
	24-h	0.721	0.765	0.718	4.511	- 5.690		1.368	196	II
Denver Conventional	3 h	0.817	0.030	0.851	0.707	- 3.831	0.0-5.33	0.402	239	II
	8-h	0.792	0.120	0.714	2.408	- 7.448		0.393	209	II
	24-h	0.662	0.186	0.542	2.944	- 7.818		0.386	112	III
Chicago Experimental I	3-h	0.951	0.305	0.899	3.532	- 5.829	1.3-16	0.769	292	II
	8-h	0.873	0.533	0.788	4.059	- 7.320		0.900	233	II
	24-h	0.949	0.286	0.845	2.809	- 6.592		0.602	144	II
Pittsburgh Low-Rise Apt. I	3-h	0.855	0.117	1.046	0.465	1.295	0.67-58.3	3.573	323	II
	8 h	0.853	-0.630	1.29	- 1.99	5.995		3.85	262	II
	24-h	0.929	0.376	1.167	-1.795	4.399		2.053	151	II
Baltimore Experimental I	3-h	0.809	0.119	0.840	1.333	- 4.469	0.0-16	1.184	290	II
	8-h	0.821	0.246	0.621	3.358	-14.007		0.921	256	III
	24-h	0.832	0.196	0.603	2.251	-13.909		0.964	201	III
Washington Conventional I	3-h	0.879	0.043	0.915	0.818	- 3.045	0.0-12.78	0.642	320	II
	8-h	0.863	0.096	0.798	1.778	- 6.830		0.518	252	II
	24-h	0.747	0.299	0.602	5.48	- 9.277		0.314	159	III
Baltimore Conventional I	3-h	0.727	0.227	0.590	6.571	-12.421	0.0-3.78	0.417	287	III
	8-h	0.677	0.198	0.533	4.500	-11.805		0.441	216	III
	24-h	0.771	0.121	0.633	2.785	- 8.270		0.376	141	III
Washington Experimental I	3-h	0.961	-0.006	0.936	- 1.07	-3.856	0.0-12	0.664	267	II
	8-h	0.942	0.006	0.886	- 0.095	-5.062		0.721	201	II
	24-h	0.984	-0.051	0.921	- 1.101	-5.008		0.395	110	II

TABLE 11. STATISTICAL DATA SUMMARY FOR METHANE (CH_4 ppm)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.914	0.352	0.769	5.246	-12.438	0.0-10.2	0.878	341	II
	8-h	0.895	0.251	0.861	3.197	- 5.50		0.917	291	II
	24-h	0.880	0.307	0.823	3.315	- 5.656		0.887	203	II
Denver Conventional	3 h	0.812	0.579	0.716	7.227	- 8.521	0.11-9.17	0.392	239	II
	8-h	0.689	0.930	0.556	9.199	-10.951		0.446	209	III
	24-h	0.708	0.813	0.576	6.25	- 7.741		0.359	112	III
Chicago Experimental I	3-h	0.921	0.086	0.931	2.629	- 3.884	0.0-3	0.198	301	II
	8-h	0.847	0.068	0.917	1.226	- 2.220		0.268	242	I
	24-h	0.844	0.120	0.840	1.734	- 3.555		0.251	144	II
Pittsburgh Low-Rise Apt. I	3-h	0.832	0.226	0.779	5.628	- 7.630	0.0-6	0.442	324	II
	8 h	0.816	0.268	0.753	5.618	- 7.469		0.460	262	II
	24-h	0.870	0.215	0.799	4.11	- 5.438		0.362	152	II
Baltimore Experimental I	3-h	0.871	0.441	0.763	7.582	- 9.364	0.78-4.9	0.380	290	II
	8-h	0.859	0.483	0.731	7.601	- 9.833		0.460	256	II
	24-h	0.850	0.474	0.723	6.080	- 8.704		0.444	201	II
Washington Conventional I	3-h	0.943	0.127	0.907	4.281	- 5.316	0.67-3.0	0.181	338	II
	8-h	0.886	0.210	0.836	4.669	- 6.182		0.253	275	II
	24-h	0.918	0.108	0.913	2.335	- 2.949		0.206	183	II
Baltimore Conventional I	3-h	0.940	0.212	1.008	0.352	1.164	1.0-18.0	1.744	289	I
	8-h	0.940	-0.332	1.141	-1.534	5.039		1.757	224	II
	24-h	0.951	-0.554	1.200	-2.222	6.027		1.664	150	II
Washington Experimental I	3-h	0.928	0.147	0.995	1.794	-0.0233	0.0-8.1	0.685	297	I
	8-h	0.919	0.179	0.986	1.898	-0.490		0.722	238	I
	24-h	0.904	0.197	0.994	1.534	-0.164		0.820	157	I

Carbon Dioxide--

The last pollutant investigated in this section is CO_2; Table 12 illustrates that the GIOAP model estimates the indoor CO_2 concentrations very well. Nine cases are judged Class II, and 15 are judged Class I. Following the procedure used in the other pollutant analysis, the difference between the estimated CO_2 concentrations and the corresponding observed indoor values is at no time greater than 8% of the observed value.

Model Sensitivity

An integral part of the model validation is a theoretical analysis of the model sensitivity. A study of this nature shows how errors in the estimation of a model parameter affect the model output(s). One of the unique features of the GIOAP model is the transient term. Previous numerical studies simulating the relative balance between the indoor and outdoor environments have included only steady-state conditions. An assessment of the transient term indicates that this term is most important for stable pollutants, but its contribution is minimal for reactive pollutants. Exclusion of the transient term reduces the correlation between observed and estimated values by about 50% of its value with the transient term included. Exclusion of the transient term does not have any effect on the estimations of indoor concentrations of the chemically reactive ozone. This behavior is expected from theoretical considerations, since for ozone the decay term in the exponent of the transient term is very large; therefore, the transient term approaches zero, which is not the case for stable pollutants. Thus the GIOAP model becomes a steady-state model for reactive pollutants; the model, however, is very sensitive to the transient term for the stable pollutants. A sensitivity analysis will further indicate which parameters are highly sensitive to errors (i.e., a small error in such a parameter would result in a significant error in the output(s)) and which parameters are relatively insensitive to errors. Knowledge of the sensitivity of the various parameters will assist us in determining priorities in the utility of the model and in estimating parameter values when the model becomes

TABLE 12. STATISTICAL DATA SUMMARY FOR CARBON DIOXIDE (CO_2 ppm)

Residence	t_{epis}	r	b	m	t_b	t_m	Range of indoor observed value	SEE	No. of observ.	Comments
Pittsburgh Mobile Home I	3-h	0.973	42.175	0.948	3.495	-4.199	464-2231	75.482	342	II
	8-h	0.929	-10.878	1.033	-0.484	1.4		115.026	296	II
	24-h	0.943	12.243	0.999	0.529	-0.027		93.16	204	II
Denver Conventional	3 h	0.837	- 5.166	1.061	-0.280	1.567	157-1587	104.417	320	I
	8-h	0.730	-35.016	1.174	-1.215	2.711		133.177	297	II
	24-h	0.656	-93.259	1.275	-1.840	2.444		132.292	172	I
Chicago Experimental I	3-h	0.948	30.654	0.953	2.389	-2.610	394-2094	61.542	322	II
	8-h	0.919	21.308	0.948	1.098	-2.025		78.768	247	I
	24-h	0.981	15.496	0.964	1.319	-2.314		39.577	148	I
Pittsburgh Low-Rise Apt. I	3-h	0.967	43.778	0.941	3.831	-4.231	351-2197	66.333	321	II
	8 h	0.953	21.220	0.986	1.334	-0.703		67.825	260	I
	24-h	0.929	43.220	0.946	1.696	-1.770		67.398	151	I
Baltimore Experimental I	3-h	0.921	35.860	0.943	2.589	-2.368	315-1384	59.053	281	II
	8-h	0.900	5.939	0.992	0.328	-0.268		66.851	238	I
	24-h	0.910	-23.461	1.051	-1.131	1.415		68.991	176	I
Washington Conventional I	3-h	0.979	12.643	0.984	1.154	-1.414	218-1679	48.819	317	I
	8-h	0.954	4.027	1.003	0.283	0.014		75.309	259	I
	24-h	0.979	18.378	0.960	1.736	-2.669		47.999	175	I
Baltimore Conventional I	3-h	0.932	21.506	0.955	2.076	-2.163	326-1463	56.075	318	I
	8-h	0.950	20.668	0.949	2.180	-2.595		44.446	257	II
	24-h	0.943	7.237	0.986	0.594	-0.549		38.916	177	I
Washington Experimental I	3-h	0.893	75.750	0.878	5.611	-4.904	0.0-1100	72.325	318	II
	8-h	0.896	41.831	0.948	2.743	-1.796		70.997	265	II
	24-h	0.905	53.971	0.908	3.160	-2.790		62.615	169	II

an application tool. Model validation studies are often undertaken under the best possible conditions; thus, it is necessary to study the model's sensitivity in order to define its limitations and capabilities.

For a given general model $y = f(\overline{X},\overline{P})$, model sensitivity is defined as:

$$\left.\frac{\partial f(\overline{X},\overline{P})}{\partial p_i}\right|_{(\overline{X},\overline{P}) = (\overline{X}_0,\overline{P}_0)} \tag{14}$$

where

f = the function defining the mathematical model

$\overline{X} = \{x_1, x_2, \ldots, x_n\}$ = the vector of independent variables

$\overline{X}_0 = \{x_{1_0}, x_{2_0}, \ldots, x_{n_0}\}$ = fixed value of $\overline{X}$

$\overline{P} = \{p_1, p_2, \ldots, p_k\}$ = the vector of parameters

$\overline{P}_0 = \{p_{1_0}, p_{2_0}, \ldots, p_{k_0}\}$ = fixed value of $\overline{P}$.

For some insight as to why this formula is used to measure model sensitivity, one should recall the following equation:

$$df = \sum_{i=1}^{k} \frac{\partial f}{\partial p_i} dp_i \tag{15}$$

Equation (15) indicates that the approximate error (df) of f is a linear combination of the errors in the individual parameters (dp_i, i=1, ..., k) where the coefficient of each dp_i, i=1, ..., k is the corresponding sensitivity coefficient. This approach is used for error or sensitivity analysis when Δf, the actual change in the function, can be approximated by df.

The GIAOP model is a first-order initial value problem given by Equation (3). Thus, for this case, the function f referred to in the definition of model sensitivity is replaced by C_{in}, Equation (4). The GIOAP model sensitivity coefficients are as follows:

$$\frac{\partial C_{in}}{\partial C_{in_0}} = e^{-(D+\nu)(t-t_0)} \qquad t_0 \le t \le t_f \tag{16}$$

$$\frac{\partial C_{in}}{\partial m_{out}} = \left(\frac{\nu}{D+\nu}\right)\left[\left(\frac{1}{D+\nu} - t_0\right)e^{-(D+\nu)(t-t_0)} - \left(\frac{1}{D+\nu} - t\right)\right] \qquad t_0 \leq t \leq t_f \tag{17}$$

$$\frac{\partial C_{in}}{\partial b_{out}} = \left(\frac{\nu}{D+\nu}\right)\left(1 - e^{-(D+\nu)(t-t_0)}\right) \qquad t_0 \leq t \leq t_f \tag{18}$$

$$\frac{\partial C_{in}}{\partial S} = \frac{1 - e^{-(D+\nu)(t-t_0)}}{V(D+\nu)} \qquad t_0 \leq t \leq t_f \tag{19}$$

$$\begin{aligned}\frac{\partial C_{in}}{\partial D} = {} & \left(\frac{1}{D+\nu}\right)^2 \left(m_{out}\nu t_0 + \nu b_{out} + \frac{S}{V} - \frac{2m_{out}\nu}{D+\nu}\right) e^{-(D+\nu)(t-t_0)} \\ & -\left[C_{in_0} - \left(\frac{1}{D+\nu}\right)\left(m_{out}\nu t_0 + \nu b_{out} + \frac{S}{V} - \frac{m_{out}\nu}{D+\nu}\right)\right](t-t_0)e^{-(D+\nu)(t-t_0)} \\ & - \left(\frac{1}{D+\nu}\right)^2 \left(\nu b_{out} + \frac{S}{V} - \frac{2m_{out}\nu}{D+\nu} + m_{out}\nu t\right) \qquad t_0 \leq t \leq t_f\end{aligned} \tag{20}$$

$$\frac{\partial C_{in}}{\partial V} = \left[\frac{S}{V^2(D+\nu)}\right]\left[e^{-(D+\nu)(t-t_0)} - 1\right] \qquad t_0 \leq t \leq t_f \tag{21}$$

$$\begin{aligned}\frac{\partial C_{in}}{\partial \nu} = {} & - \left(\frac{1}{D+\nu}\right)^2 \left[m_{out}Dt_0 + b_{out}D - \frac{S}{V} - m_{out}\left(\frac{D-\nu}{D+\nu}\right)\right]e^{-(D+\nu)(t-t_0)} \\ & -\left[C_{in_0} - \left(\frac{1}{D+\nu}\right)\left(m_{out}\nu t_0 + b_{out}\nu + \frac{S}{V} - \frac{m_{out}\nu}{D+\nu}\right)\right](t-t_0)e^{-(D+\nu)(t-t_0)} \\ & + \left(\frac{1}{D+\nu}\right)^2 \left[b_{out}D - \frac{S}{V} - m_{out}\left(\frac{D-\nu}{D+\nu}\right) + m_{out}Dt\right] \qquad t_0 \leq t \leq t_f\end{aligned} \tag{22}$$

where

t_0 = initial time

t_f = final time.

In the balance of this document the subscripts referring to indoors and outdoors will be eliminated; thus, we will denote C_{in_0} by C_0, C_{in} by C, m_{out} by m, and b_{out} by b.

The study documented in this report requires several additional, though nonrestrictive, assumpsions to be made (see Section 2) in order to implement the model, Equation (4). These assumptions resulted in Equation (5). The sensitivity coefficients for Equation (5) are as follows (see Appendix A for the derivations of the sensitivity coefficients):

$$\frac{\partial C_m}{\partial C_0} = e^{-\sum_{i=1}^{m} (\nu_i+D_i)} \tag{23}$$

$$\frac{\partial C_m}{\partial m_i} = \alpha_i \left\{ \left(\frac{\nu_i}{D_i+\nu_i}\right) \left[\left(\frac{1}{D_i+\nu_i} - t_{i-1}\right) e^{-(\nu_i+D_i)} - \left(\frac{1}{D_i+\nu_i} - t_i\right) \right] \right\} \tag{24}$$

$$\frac{\partial C_m}{\partial b_i} = \alpha_i \left(\frac{\nu_i}{D_i+\nu_i}\right) \left(1 - e^{-(\nu_i+D_i)}\right) \tag{25}$$

$$\frac{\partial C_m}{\partial S_i} = \alpha_i \left[\frac{1 - e^{-(\nu_i+D_i)}}{V(\nu_i+D_i)} \right] \tag{26}$$

$$\frac{\partial C_m}{\partial D_i} = \alpha_i \Bigg\{ \left(\frac{1}{D_i+\nu_i}\right)^2 \left[m_i \nu_i t_{i-1} + \nu_i b_i + \frac{S_i}{V} - \frac{2m_i\nu_i}{D_i+\nu_i}\right] e^{-(\nu_i+D_i)}$$

$$- \left[C_{i-1} - \left(\frac{1}{D_i+\nu_i}\right)\left(m_i\nu_i t_{i-1} + \nu_i b_i + \frac{S_i}{V} - \frac{m_i\nu_i}{D_i+\nu_i}\right)\right] e^{-(\nu_i+D_i)}$$

$$- \left(\frac{1}{D_i+\nu_i}\right)^2 \left(\nu_i b_i + \frac{S_i}{V} - \frac{2m_i\nu_i}{D_i+\nu_i} + m_i\nu_i t_i\right)\Bigg\} \tag{27}$$

$$\frac{\partial C_m}{\partial V} = \alpha_i \left[\frac{S_i}{V^2(D_i+\nu_i)}\right]\left(e^{-(\nu_i+D_i)} - 1\right) \tag{28}$$

$$\frac{\partial C_m}{\partial \nu_i} = \alpha_i \Bigg\{ - \left(\frac{1}{D_i+\nu_i}\right)^2 \left[m_i D_i t_{i-1} + b_i D_i - \frac{S_i}{V} - m_i\left(\frac{D_i-\nu_i}{D_i+\nu_i}\right)\right] e^{-(\nu_i+D_i)}$$

$$- \left[C_{i-1} - \left(\frac{1}{D_i+\nu_i}\right)\left(m_i\nu_i t_{i-1} + b_i \nu_i + \frac{S_i}{V} - \frac{m_i\nu_i}{D_i+\nu_i}\right)\right] e^{-(\nu_i+D_i)}$$

$$+ \left(\frac{1}{D_i+\nu_i}\right)^2 \left[b_i D_i - \frac{S_i}{V} - m_i\left(\frac{D_i-\nu_i}{D_i+\nu_i}\right) + m_i D_i t_i\right]\Bigg\} \tag{29}$$

where

$$\frac{\partial C_m}{\partial(\ )} = \frac{\partial C}{\partial(\ )}\Bigg|_{(t_m,\ m_m,\ b_m,\ S_m,\ D_m,\ V,\ \nu_m,\ C_{m-1})}$$

$(\ )$ = any one of the GIOAP model parameters

$t_0 \le t_i,\ t_m \le t_n = t_f,\ 1 \le i,\ m \le n$

$$\alpha_i = \begin{cases} 1, & i = m \\ e^{-\sum\limits_{j=i+1}^{m} (\nu_j+D_j)}, & 1 \le i < m \end{cases}$$

Two major advantages become apparent when the closed form partial derivatives are available. The first is the ease with which the sensitivity coefficients can be computed. The second is that the sensitivity coefficients can be given a thorough analytical treatment which is difficult, if not impossible, when the partial derivatives are not available in closed form. Each of the seven sensitivity coefficients (Equations (23) through (29)) will be discussed below.

The first sensitivity coefficient to be considered is $\partial C_m/\partial C_0$. Referring back to Equation (23), it is seen that $0 < \partial C_m/\partial C_0 < 1$. Moreover, as time increases, $\partial C_m/\partial C_0$ decreases, which means that the effect of an error in C_0 on C diminishes with time. Finally, since $\partial C_m/\partial C_0$ is positive, an increase in C_0 will cause an increase in C_m, and a decrease in C_0 will result in a decrease in C_m.

Next, the sensitivity coefficients involving m, the slope of the line used to approximate the outdoor pollutant concentrations, will be dealt with. By rearranging and deleting terms from Equation (24), it is seen that

$$0 \leq \left|\frac{\partial C_m}{\partial m_i}\right| < \alpha_i \quad \frac{\nu_i}{D_i+\nu_i} \quad t_i, \qquad 1 \leq i, m \leq n \quad . \tag{30}$$

Equation (30) shows that the effects on C of an error in m at $t = t_i$ will dissipate with time. On the other hand, it should be noted that if there is a recurrent error in m (e.g., every value of m_i, i = 1, ..., n is in error by 20%, the effects will be additive (see Appendix A), i.e.,

$$dC_\ell = \sum_{i=1}^{m} \frac{\partial C_\ell}{\partial m_i} dm_i, \quad \ell = 1, \ldots, n \tag{31}$$

with the elements having the lowest indices contributing less and less to the error in C.

The sensitivity coefficients involving b, the intercept of the line used to approximate the outdoor pollutant concentrations, will be examined in this paragraph. From Equation (25), it is clear that

$$0 < \frac{\partial C_m}{\partial b_i} < \alpha_i \left(\frac{\nu_i}{D_i+\nu_i}\right), \qquad 1 \le i, m \le n \ . \tag{32}$$

Thus, the effects of an error in b at t_i on C diminish with time. Also, $\partial C_m/\partial b_i \le 1$, which means that errors in b are not magnified when they are transmitted to C. In addition, the fact that $\partial C_m/\partial b_i$ is positive means that an increase in b_i causes an increase in C_m, and, similarly, a decrease in b_i results in a decrease in C_m. As in the case of m, recurrent errors in b are additive.

The sensitivity coefficients involving S, the internal pollutant source rate, will be discussed next. It is seen from Equation (26) that

$$0 < \frac{\partial C_m}{\partial S_i} < \frac{\alpha_i}{V(\nu_i+D_i)} \ , \qquad 1 \le i, m \le n \ . \tag{33}$$

As before, due to the action of α_i, the effects of an error in S at t_i on C will decrease with time. In addition, considering the fact that V is a large number and that the product V times ν + D is large (even though ν is usually in the interval (0.1, 2.0)), it is seen that $\partial C_m/\partial S_i$ will be small. Thus, C is relatively insensitive to errors in S. Moreover, since $\partial C_m/\partial S_i$ is positive, it is seen that an increase (decrease) in S_i will result in an increase (decrease) in C_m. Finally, as in the case of m, recurrent errors in S are additive.

The next sensitivity coefficients to be studied are those that deal with chemical decay rate, D. From Equation (27) it is seen that the expression for $\partial C_m/\partial D_i$ is a very complicated one. As a result, it is hard to make any meaningful analysis or calculate any useful bounds. As before, the effects of an error in ν_i at $t = t_i$ will diminish with time, and the effects of recurrent errors are additive.

The next sensitivity coefficient to be examined is $\partial C_m/\partial V$. Since V does not change from hour to hour, any error associated with V will occur initially and will dissipate with time as in the case of C_0. Also, it is easily seen from Equation (28) that $\partial C_m/\partial V$ is less than zero. Thus, an increase (decrease) in V would cause a decrease (increase) in C_m. Values of V are usually obtainable from plans or blueprints, thus minimizing any error connected with V; thus V is, for all practical purposes, a known constant, and $\partial C_m/\partial V$ was presented here as a point of interest.

Finally, the sensitivity coefficients associated with the air exchange rate ν will be discussed. As can be seen from Equation (29), $\partial C_m/\partial V_i$ is a complex expression, and, due to the interactions of the various elements of the equation, it is difficult to make any meaningful analysis or to compute any useful bounds. As in previous cases, the effects of an error in ν_i at $t = t_i$ on C will diminish with time, and the effects of recurrent errors are additive.

The balance of this section will consist of graphical illustrations representing the effects induced on the indoor pollutant concentrations by errors imposed on different input parameters. Figure 8 represents the nominal conditions, i.e., a carbon monoxide (CO) 8-h episode calculated by the GIOAP model; this episode is extracted from the data set of the Baltimore Conventional Residence, Visit Number 1. The baseline conditions are also shown in Table 13.

Figure 9 shows how a 50% error on the initial condition affects C_{in} over the 8-h episode. The figure illustrates that for this example the effects of the initial condition error on the indoor concentration are essentially eliminated after 2 h. This case is an example of a nonrecurrent error; i.e., a single parameter is perturbed only once in the episode, and the effects of the introduced perturbation are traced for the duration of the episode. The same type of error behavior in C_{in} seen in this example will occur for any other parameter under similar conditions.

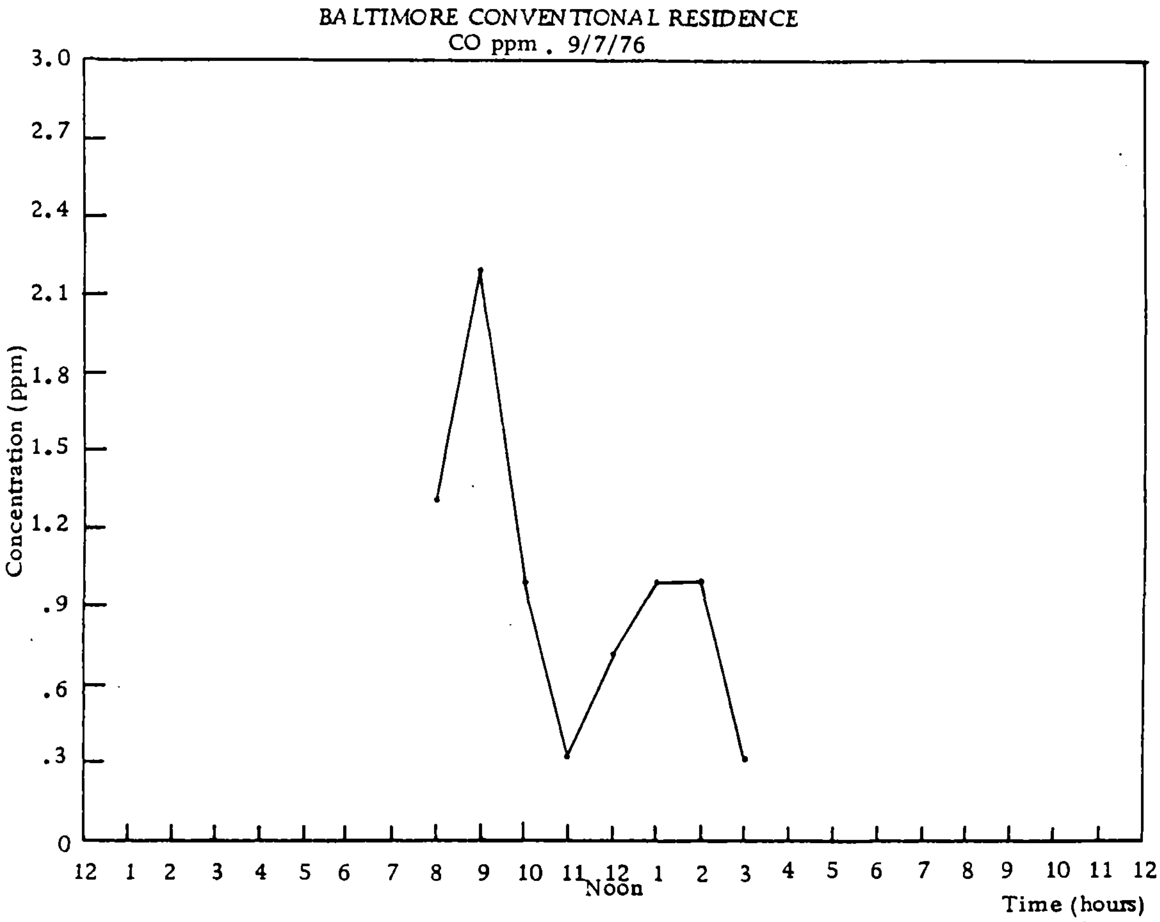

Figure 8. Nominal values.

TABLE 13. NOMINAL CONDITIONS USED IN THE SENSITIVITY STUDY EXAMPLES

House: Baltimore Conventional (Visit #1)
Pollutant: CO
Volume: 13,575 ft^3

Hour	C_{in} (ppm)	C_{out} (ppm)	S (mg/h)	ν (air exchanges/h)
8	1.33	1.33	-	-
9	2.23	1.33	677.77	1.20
10	1.04	0.00	0.00	1.20
11	0.31	0.00	0.00	1.20
12	0.68	0.00	440.14	1.20
13	1.02	0.00	613.13	1.20
14	1.01	0.00	528.17	1.20
15	0.30	0.00	0.00	1.20

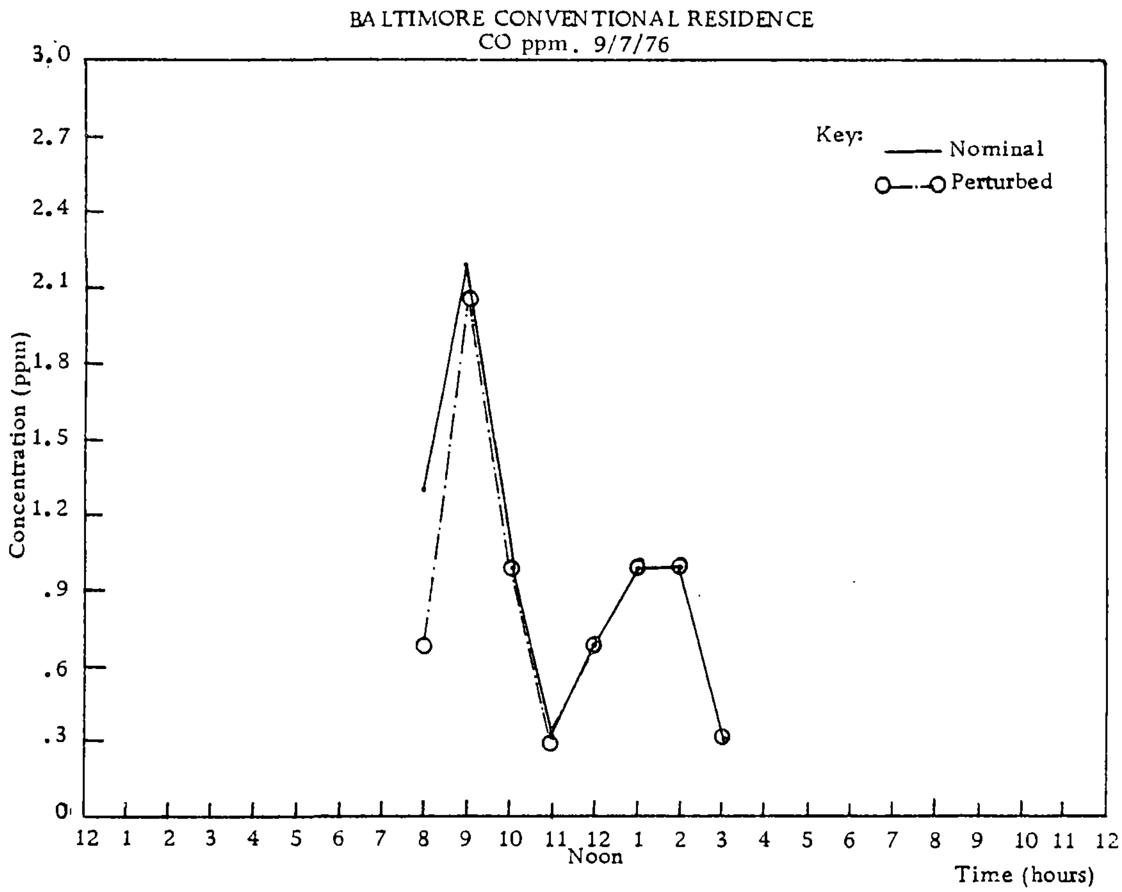

Figure 9. Comparison of nominal values obtained by perturbing C_{in}.

Figure 10 illustrates the errors in the indoor pollutant levels caused by recurrent time-dependent errors in the internal source (S) rate term. The magnitude of the error in S at a given time is 30% of the corresponding internal source rate.

Figure 11 illustrates the errors in the indoor pollutant level caused by a recurrent constant error in the air exchange rate (ν). The nominal input value for ν is 1.2 air exchanges per hour, the error used is 0.2 air exchanges per hour.

Numerical investigations of the above illustrated cases appear in Appendix B, where the sensitivity coefficients, the parameter errors (ΔS, $\Delta\nu$, ΔC_0), the actual output errors (ΔC_{in}), and approximate output errors (dC_{in}) are tabulated.

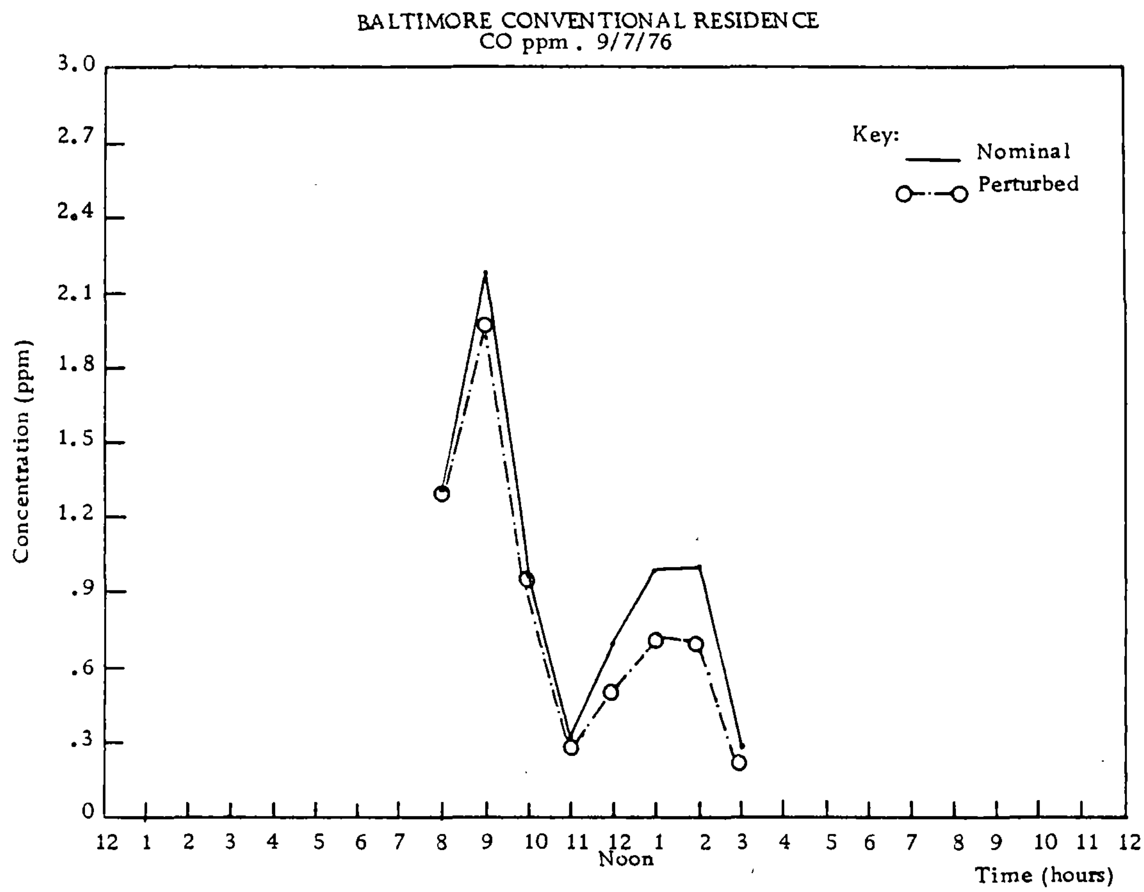

Figure 10. Comparison of nominal values with values obtained by perturbing S.

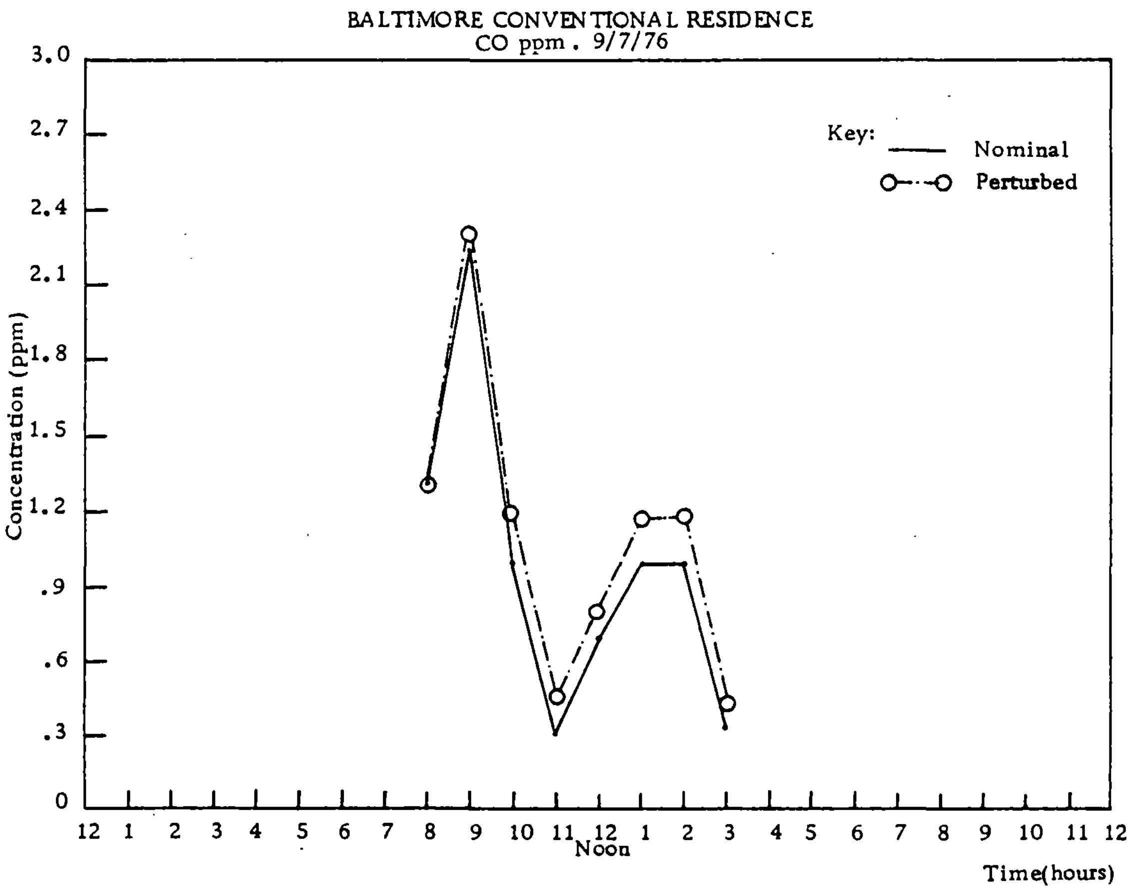

Figure 11. Comparison of nominal values with values obtained by perturbing υ.

SECTION 4

CONCLUSIONS

This study indicates that the GIOAP model performs well. The fundamental principles and assumptions used in the formulation of the GIOAP model are similar to the concepts used for other indoor numerical models; however, the GIOAP model is different from previous numerical efforts because it is applicable to, and has been applied to, a large variety of pollutants and because it simulates short periods of time since the transient term is included. Most importantly, the GIOAP model stands alone because it is the only indoor-outdoor numerical model that has been validated against a large set of observed data.

The GIOAP model has been tested under a wide variety of meteorological and behavioral conditions. Weather conditions encountered ranged from late autumn in Denver to summer in Baltimore to winter in Pittsburgh. Behavioral patterns varied widely, e.g., families with children versus families without children, and families with smoking members versus nonsmoking families. In addition the GIOAP has simulated conditions in residences of different structural characteristics, e.g., detached dwellings, row houses, apartments, and mobile homes. Thus, not only does the GIOAP model provide good estimates of indoor air pollutant concentration levels for different pollutants, but also it does so for various types of residential structures under diverse meteorological and behavioral conditions.

The transient term included in the GIOAP model does not appear in other numerical models that estimate indoor air pollution levels. Examination of the GIOAP model and simulations with and without the transient term have led to the following conclusions: (a) the transient term contributes substantially when the variation of indoor concentrations for stable pollutants is simulated; (b) the transient term becomes less significant for moderately reactive pollutants; and (c) the transient term is unimportant for ozone which is a highly reactive pollutant.

The model validation phase was undertaken under "best" conditions, i.e., the parameter values used for simulation were the best estimates available. For C_0, m, b, and V the actual values were obtained from the monitoring data. The large data base available for this study was utilized to compute constrained best least-squares estimates for S and ν, the two parameters most difficult to obtain. The estimates for these two parameters were computed with the Parameter Estimation Procedure (PEP) (see Section 3). Finally, values for D for various pollutants were obtained from the available literature.

The motivation for obtaining the "best" estimates for all the parameters underscores our desire to validate the GIOAP model under ideal conditions, to characterize its performance without considering the problems of obtaining realistic values for the input parameters, and subsequently, to determine its sensitivity resulting from errors in the values of the input parameters.

The GIOAP model was statistically tested using two set of rules: (a) strict statistical tests, and (b) predetermined empirical criteria. Under "best" conditions, the model performance is divided into three categories:

1. Not Validated--Due to low outdoor levels and a negative interference of CO_2 on the SO_2 monitor, a large number of hourly sulfur dioxide concentrations are measured close to the threshold value of the monitor. In the indoor environment SO_2 and NO_2 have an approximately equal half-life; it is thus judged that the GIOAP model would validate satisfactorily against higher indoor SO_2 concentrations.

2. Adequate--Eighty-five percent of the observed indoor ozone values are in the low range of 0-6 ppb. The model estimated values are mostly within 2 ppb (less than the instrument precision) of the observed values. The numerical output does not satisfy the predetermined model validation criteria, but it provides realistic estimations of the indoor ozone concentrations.

3. Satisfactory--Model estimated values are within 25% of the observed indoor values for the following pollutants: CO, NO, NMHC, CH_4, CO_2, and NO_2.

Under "best" conditions the GIOAP model provides realistic estimates of the observed indoor pollutant concentrations. However, due to the nature of the model usage, it is necessary to investigate the performance of the model under less than ideal conditions. As a result, a sensitivity study of the GIOAP model is necessary. The set of parameters associated with the GIOAP model has been divided into two groups: (a) those parameters that remain constant throughout an episode (C_0, V), and (b) those that must be estimated for every hour of the episode (m, b, S, ν, D).

The model is comparatively insensitive with respect to parameters in the first group, i.e., errors in C_0 and V have relatively little effect on the model output. In addition, the effects of errors in C_0 and V dissipate with time (see Section 3). Errors in the second group have more impact on the model output. This is due to two factors: (a) estimates of parameter values in this group are more susceptible to error than are the parameters in the first group, and (b) errors can be introduced at each hour of the episode because these parameters must be estimated every hour. In an effort to stratify the parameters of this group on a relative basis, they are ranked as follows from the least to the most sensitive: (1) S, (2) b, and (3) D, m and ν. S is the least sensitive due to the fact that the magnitude of the numerator is less than one, and the denominator, which contains a factor of V, is relatively large. b is considered to be somewhat more sensitive than S due to the fact that $\partial C/\partial S = (1/\nu V)(\partial C/\partial b)$ and that, within the range of values being used, $1/\nu V$ is less than 1. Finally, D, m, and ν are considered to be the most sensitive, even though the complexity of their respective sensitivity coefficients does not allow any general conclusions to be drawn. Intuition and the examples studied suggest that these are the three most sensitive parameters.

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APPENDIX A

DERIVATION OF THE GIOAP MODEL SENSITIVITY COEFFICIENTS

As stated in the text, a sensitivity study involves analyzing the change in the output(s) of a model resulting from a change in the parameter(s). When a function such as

$$y_i = f(t_i, \overline{P}) \tag{A-1}$$

where

t_i = time, $i = 1, \ldots, n$

$\overline{P} = \{p_1, \ldots, p_k\}$ = vector of parameters

$\overline{P}_0 = \{p_{1_0}, \ldots, p_{k_0}\}$ = fixed value of $\overline{P}$

is to undergo a sensitivity analysis, the procedure is straightforward: evaluate the first partial derivatives of f with respect to the parameter(s) at a specified condition (i.e., $\partial f/\partial p_j \big|_{(t_i, \overline{P}_0)}$, $j = 1, \ldots, k$) in order to determine how variations in the parameter(s) affect the output. However, when the function is of the form

$$y_i = f(t_i, \overline{P}_i, y_{i-1}) \tag{A-2}$$

where

t_i = time, $i = 1, \ldots, n$

y_0 = initial value of the output variable

$\overline{P}_i = \overline{P}(t_i) = \{p_{1i}, \ldots, p_{ki}\}$, $i = 1, \ldots, n$ = vector of time-dependent parameters

$\overline{P}_{i_0} = \{p_{1i_0}, \ldots, p_{ki_0}\}$ = fixed value of $\overline{P}_i$, $i = 1, \ldots, n$

the analysis becomes considerably more involved. This is due to the fact that at $t = t_i$, f is not only a function of $\overline{P}_i$ but also of all the previous parameter vectors, $\overline{P}_j$, $j = 1, \ldots, i-1$, and y_0 as a result of the dependence on y_{i-1}. Thus, the sensitivity coefficients that must be determined are

$$\left.\frac{\partial f}{\partial y_0}\right| (t_j, \overline{P}_{j_0}, y_{j-1}) \quad j = 1, \ldots, n \tag{A-3}$$

$$\left.\frac{\partial f}{\partial p_i}\right| (t_j, \overline{P}_{j_0}, y_{j-1}) \quad i = 1, \ldots, k, \; j = 1, \ldots, n \tag{A-4}$$

The sensitivity coefficients will be derived below by first obtaining a general expression for the total differential, then taking the sensitivity coefficients to be the coefficients of the parameter differentials. Before the derivation of the sensitivity coefficients for Equation (A-2) can be developed, the following additional notation is required.

$d\overline{P}_i = d\overline{P}(t_i) = (dp_{1i}, \ldots, dp_{ki}),\ i = 1, \ldots, n$ = vector of time-dependent parameter variations

$d\overline{P}_{i_0} = (dp_{1i_0}, \ldots, dp_{ki_0})$ = fixed value of $d\overline{P}_i$, $i = 1, \ldots, n$

dy_i = the change in the dependent variable at time, t_i, $i = 1, \ldots, n$, due to a change in the parameter(s)

$$\frac{\partial y_i}{\partial \overline{P}_i} = \left(\left.\frac{\partial f}{\partial p_j}\right| (t_i, \overline{P}_{i_0}, y_{i-1}),\ j = 1, \ldots, k\right)$$

= the vector of partial derivatives of the function with respect to the parameter(s) evaluated at $(t_i, \overline{P}_{i_0}, y_{i-1})$

$$\frac{\partial y_i}{\partial y_{i-1}} = \left.\frac{\partial f}{\partial y_{i-1}}\right| (t_i, \overline{P}_{i_0}, y_{i-1})$$

$$\frac{\partial y_i}{\partial \overline{P}_i} \cdot d\overline{P}_{i_0} = \sum_{j=1}^{k} \left(\left.\frac{\partial f}{\partial p_j}\right| (t_i, \overline{P}_{i_0}, y_{i-1})\right) dp_{ji_0}$$

= the dot product of the two vectors, $\partial y_i/\partial \overline{P}_i$ and $d\overline{P}_{i_0}$.

The general expression for dy_m, $1 \leq m \leq n$, is derived in the following set of equations:

$$dy_1 = \frac{\partial y_1}{\partial y_0} dy_0 + \frac{\partial y_1}{\partial \overline{P}_1} \cdot d\overline{P}_{1_0} \tag{A-5}$$

$$dy_2 = \frac{\partial y_2}{\partial y_1} dy_1 + \frac{\partial y_2}{\partial \overline{P}_2} \cdot d\overline{P}_{2_0} = \frac{\partial y_2}{\partial y_1} \frac{\partial y_1}{\partial y_0} dy_0$$

$$+ \frac{\partial y_2}{\partial y_1} \frac{\partial y_1}{\partial \overline{P}_1} \cdot d\overline{P}_{1_0} + \frac{\partial y_2}{\partial \overline{P}_2} \cdot d\overline{P}_{2_0} \tag{A-6}$$

$$dy_3 = \frac{\partial y_3}{\partial y_2} dy_2 + \frac{\partial y_3}{\partial \overline{P}_3} \cdot d\overline{P}_{3_0} = \frac{\partial y_3}{\partial y_2} \frac{\partial y_2}{\partial y_1} \frac{\partial y_1}{\partial y_0} dy_0$$

$$+ \frac{\partial y_3}{\partial y_2} \frac{\partial y_2}{\partial y_1} \frac{\partial y_1}{\partial \overline{P}_1} \cdot d\overline{P}_{1_0} + \frac{\partial y_3}{\partial y_2} \frac{\partial y_2}{\partial \overline{P}_2} \cdot d\overline{P}_{2_0} + \frac{\partial y_3}{\partial \overline{P}_3} \cdot d\overline{P}_{3_0} \tag{A-7}$$

$$\vdots$$

$$dy_m = \left(\prod_{i=1}^{m} \frac{\partial y_i}{\partial y_{i-1}} \right) dy_0 + \sum_{i=1}^{m-1} \left(\prod_{j=i+1}^{m} \frac{\partial y_j}{\partial y_{j-1}} \right) \frac{\partial y_i}{\partial \overline{P}_i} \cdot d\overline{P}_{i_0}$$

$$+ \frac{\partial y_m}{\partial \overline{P}_m} \cdot d\overline{P}_{m_0} \; . \tag{A-8}$$

In order to obtain the coefficients of the parameter differentials, we expand the dot products in Equation (A-8)

$$dy_m = \left(\prod_{i=1}^{m} \frac{\partial y_i}{\partial y_{i-1}}\right) dy_0 + \sum_{\ell=1}^{k} \sum_{i=1}^{m-1} \left(\prod_{j=i+1}^{m} \frac{\partial y_j}{\partial y_{j-1}}\right) \left(\frac{\partial f}{\partial p_\ell} \bigg| \ (t_i,\ \overline{P}_{i_0},\ y_{i-1})\right) dp_{\ell i_0}$$

$$+ \sum_{\ell=1}^{k} \left(\frac{\partial f}{\partial p_\ell} \bigg| \ (t_m,\ \overline{P}_{m_0},\ y_{m-1})\right) dp_{\ell m_0} \quad . \qquad \text{(A-9)}$$

Now the desired sensitivity coefficients may be easily obtained from equation (A-9). For a given value of m, $1 \leq m \leq n$, the sensitivity coefficients are as follows:

$$\frac{\partial f}{\partial y_0} \bigg| \ (t_m,\ \overline{P}_{m_0},\ y_{m-1}) = \prod_{i=1}^{m} \frac{\partial y_i}{\partial y_{i-1}} \qquad \text{(A-10)}$$

$$\frac{\partial f}{\partial p_i} \bigg| \ (t_m,\ \overline{P}_{m_0},\ y_{m-1}) = \alpha_j \left(\frac{\partial f}{\partial p_i} \bigg| \ (t_j,\ \overline{P}_{j_0},\ y_{j-1})\right) \quad i = 1,\ \ldots,\ k$$

$$j = 1,\ \ldots,\ n \qquad \text{(A-11)}$$

where

$$\alpha_j = \begin{cases} 1, \ j = m \\ \displaystyle\prod_{\ell=j+1}^{m} \frac{\partial y_\ell}{\partial y_{\ell-1}} \quad 1 \leq j < m \end{cases} \quad .$$

As mentioned previously, at $t = t_m$, f is a function of y_0 and $\overline{P}_i$, i = 1, ..., m. Equation (A-10) illustrates this dependence on y_0 and shows how an error in y_0 is propagated throughout the time period being modeled.

Similarly, Equation (A-11) for $j = 1, \ldots, m-1$ illustrates the dependence of f on past parameter vectors and shows how an error in a parameter is propagated: at the time the error appears, the change in the dependent variable is due to the change in the parameter; however, at subsequent points in time, this error is manifested as a change in the dependent variable resulting from a change in the y_{j-1} term. Finally, Equation (A-11) at $j = m$ shows that, when an initial error occurs in a parameter, the change in the dependent variable is due only to the parameter error.

In order to apply Equations (A-10) and (A-11) to the GIOAP model, let $t_j = t_f$, $t_{j-1} = t_0$, and evaluate the expressions defined by Equations (4) and (16) through (22) of Section 2 at $t = t_f$. Equation (A-10), when applied to the GIOAP model at $t = t_m$, $1 \leq m \leq n$, becomes

$$\frac{\partial f}{\partial C_0}\bigg|\,(t_m, m_m, b_m, S_m, D_m, V, \nu_m, C_{m-1}) = e^{-\sum_{i=1}^{m}(\nu_i+D_i)} \qquad \text{(A-12)}$$

Similarly, the following sensitivity coefficients are obtained by applying Equation (A-11) at $t = t_m$ to Equations (17) through (22):

$$\frac{\partial f}{\partial m_i}\bigg|\,(t_m, m_m, b_m, S_m, D_m, V, \nu_m, C_{m-1}) =$$

$$\alpha_i \left\{\left(\frac{\nu_i}{D_i+\nu_i}\right)\left[\left(\frac{1}{D_i+\nu_i} - t_{i-1}\right)e^{-(\nu_i+D_i)} - \left(\frac{1}{D_i+\nu_i} - t_i\right)\right]\right\} \qquad \text{(A-13)}$$

$$\frac{\partial f}{\partial b_i}\bigg|\,(t_m, m_m, b_m, S_m, D_m, V, \nu_m, C_{m-1}) = \alpha_i \left(\frac{\nu_i}{D_i+\nu_i}\right)\left(1 - e^{-(\nu_i+D_i)}\right) \qquad \text{(A-14)}$$

$$\frac{\partial f}{\partial S_i}\Bigg|\,(t_m,\ m_m,\ b_m,\ S_m,\ D_m,\ V,\ \nu_m,\ C_{m-1}) = \alpha_i\left[\frac{1-e^{-(\nu_i+D_i)}}{V(\nu_i+D_i)}\right] \tag{A-15}$$

$$\frac{\partial f}{\partial D_i}\Bigg|\,(t_m,\ m_m,\ b_m,\ S_m,\ D_m,\ V,\ \nu_m,\ C_{m-1}) =$$

$$\alpha_i\left\{\left(\frac{1}{D_i+\nu_i}\right)^2\left[m_i\nu_i t_{i-1} + \nu_i b_i + \frac{S_i}{V} - \frac{2m_i\nu_i}{D_i+\nu_i}\right]e^{-(\nu_i+D_i)}\right.$$

$$-\left[C_{i-1} - \left(\frac{1}{D_i+\nu_i}\right)\left(m_i\nu_i t_{i-1} + \nu_i b_i + \frac{S_i}{V} - \frac{m_i\nu_i}{D_i+\nu_i}\right)\right]e^{-(\nu_i+D_i)}$$

$$\left.-\left(\frac{1}{D_i+\nu_i}\right)^2\left(\nu_i b_i + \frac{S_i}{V} - \frac{2m_i\nu_i}{D_i+\nu_i} + m_i\nu_i t_i\right)\right\} \tag{A-16}$$

$$\frac{\partial f}{\partial V}\Bigg|\,(t_m,\ m_m,\ b_m,\ S_m,\ D_m,\ V,\ \nu_m,\ C_{m-1}) = \alpha_i\left[\frac{S_i}{V^2(D_i+\nu_i)}\right]\left[e^{-(\nu_i+D_i)} - 1\right] \tag{A-17}$$

$$\frac{\partial f}{\partial \nu_i}\Bigg|\,(t_m,\ m_m;\ b_m,\ S_m,\ D_m,\ V,\ \nu_m,\ C_{m-1}) =$$

$$\alpha_i\left\{-\left(\frac{1}{D_i+\nu_i}\right)^2\left[m_i D_i t_{i-1} + b_i D_i - \frac{S_i}{V} - m_i\left(\frac{D_i-\nu_i}{D_i+\nu_i}\right)\right]e^{-(\nu_i+D_i)}\right.$$

$$-\left[C_{i-1} - \left(\frac{1}{D_i+\nu_i}\right)\left(m_i\nu_i t_{i-1} + b_i\nu_i + \frac{S_i}{V} - \frac{m_i\nu_i}{D_i+\nu_i}\right)\right]e^{-(\nu_i+D_i)}$$

$$\left.+\left(\frac{1}{D_i+\nu_i}\right)^2\left[b_i D_i - \frac{S_i}{V} - m_i\left(\frac{D_i-\nu_i}{D_i+\nu_i}\right) + m_i D_i t_i\right]\right\} \tag{A-18}$$

APPENDIX B

NUMERICAL SENSITIVITY ANALYSIS EXAMPLES FOR THE GIOAP MODEL

In this appendix, three examples are presented which will illustrate the use of the sensitivity coefficients given in Section 3 of this report. The data used in these examples are taken from actual model calculations (CO data for the Baltimore Conventional House, first visit, hours 8-15). Table B-1 gives the nominal values for all parameters used in the examples.

TABLE B-1. NOMINAL CONDITIONS USED IN THE SENSITIVITY STUDY EXAMPLES

House: Baltimore Conventional (Visit #1)
Pollutant: CO
Volume: 13,575 ft^3

Hour	C_{in} (ppm)	C_{out} (ppm)	S (mg/h)	ν (air exchanges/h)
8	1.33	1.33	-	-
9	2.23	1.33	677.77	1.20
10	1.04	0.00	0.00	1.20
11	0.31	0.00	0.00	1.20
12	0.68	0.00	440.14	1.20
13	1.02	0.00	619.13	1.20
14	1.01	0.00	528.17	1.20
15	0.30	0.00	0.00	1.20

The first example deals with the case in which an error is made when a parameter value is estimated initially, but, after that initial error, no other errors are introduced. This situation is most likely to arise in the estimation of the initial indoor air pollutant concentration, C_0, because it is estimated only once unlike some other parameters (e.g., S and ν) which must be estimated for each hour. Using Equation (23), Table B-2 gives the approximate error (dC_{in}) and actual error (ΔC_{in}) for each hour due to an error in C_0. Here it should be noted that, since the GIOAP model is a linear function of C_0, $dC_{in} = \Delta C_{in}$; however, this does not show up in some of the entries in the table due to the fact that some values were rounded off. As mentioned in Section 3, since the sign of $\partial C_{in}/\partial C_{in_0}$ is positive, a decrease (increase) in C_0 will cause a decrease (increase) in C which can be seen in Table B-2. Finally, for this particular case, it is seen that by the 11th hour the effects of the error in C_0 on C are minimal.

TABLE B-2. ERRORS IN C_{in} DUE TO AN ERROR IN C_{in_0}

House: Baltimore Conventional (Visit #1)
Pollutant: CO

Hour	ΔC_{in_0} (ppm)	$\frac{\partial C_{in}}{\partial C_{in_0}}$	dC_{in} (ppm)	ΔC_{in} (ppm)
8	-0.665	-	-	-
9	0.000	0.3012	-0.2003	-0.20
10	0.000	0.0907	-0.0603	-0.06
11	0.000	0.0273	-0.0182	-0.01
12	0.000	0.0082	-0.0055	-0.01
13	0.000	0.0025	-0.0016	0.00
14	0.000	0.0007	-0.0005	0.00
15	0.000	0.0002	-0.0001	0.00

The next example deals with the case in which the parameter errors vary with time and are recurrent. This situation can occur in any number of the GIOAP parameters (e.g., m, b, and ν) which must be estimated. For this example the internal source rate parameter (S) was chosen, and $\Delta S_i = - 0.3\ S_i$, i = 9, ..., 15 (i.e., a negative 30% error in S). The data for this example are presented in Table B-3. Here, as in the previous example, $dC_{in} = \Delta C_{in}$ because the GIOAP model is linear with respect to S. As pointed out in Section 3, the sign of $\partial C_{in}/\partial S$ is positive; thus a decrease (increase) in S results in a decrease (increase) in C_{in}. This is illustrated in Table B-3. Also, the error term consists not only of the error due to the current perturbation of S but also of the error due to the past perturbations of S which are transmitted via the C_{i-1} term (see Equation (5)). Notice that during hours 9 through 11, the situation is similar to that of the previous example (i.e., an initial error with no errors introduced subsequently) and that the effect of the error in S has diminished by the 11th hour. However, during hours 12 through 14, errors in S occur each hour so, even though the effects of previous errors in S begin to dissipate, the overall error in C_{in} is not reduced appreciably.

TABLE B-3. ERRORS IN C_{in} DUE TO ERRORS IN S

House: Baltimore Conventional (Visit #1)
Pollutant: CO

Hour	ΔS (mg/h)	$\frac{\partial C_{in}}{\partial S}$ (ppm/mg/h)	$\frac{\partial C_{in}}{\partial C_{in_0}}$	dC_{in}* (ppm)	ΔC_{in} (ppm)
8	-	-	-	-	-
9	-203.331	0.0015	-	-0.2690	-0.27
10	0.000	0.0015	0.3012	-0.0810	-0.08
11	0.000	0.0015	0.3012	-0.0244	-0.02
12	-132.042	0.0015	0.3012	-0.1820	-0.18
13	-185.739	0.0015	0.3012	-0.3005	-0.30
14	-158.451	0.0015	0.3012	-0.3001	-0.30
15	0.000	0.0015	0.3012	-0.0904	-0.09

* In these tables, dC_{in} (Col. 5) was computed using the following formula:

$$dC_i = \underbrace{\frac{\partial C_i}{\partial C_{i-1}}}_{\text{Col. 4}} \underbrace{dC_{i-1}}_{\text{Col. 5}} + \underbrace{\frac{\partial C_i}{\partial S_i}}_{\text{Col. 3}} \underbrace{dS_i}_{\text{Col. 2}}, \quad i = 9, \ldots, 15$$

This formula is an equivalent form of equation (A-8) (see Appendix A). Also, it should be noted that any attempt to calculate dC_{in} from its components appears to result in an error. Actually, some of the values were obtained via computer and were rounded off when entered in the table.

The final example illustrates two cases: (a) that of a recurrent constant error, and (b) that in which the GIOAP model is not a linear function of the parameter being considered. The parameter being dealt with here is the air exchange rate (ν). Table B-4 presents the data associated with this example. In this example, as opposed to the previous one, the error ($\Delta\nu$ = 0.20) occurs every hour, thus the error induced in C_{in} does not have a chance to dissipate. Also, this case gives an idea of how well dC_{in} approximates ΔC_{in} when the model is not linear in the parameter being studied. Here, the approximation is fair since dC_{in}, in most cases, agrees with ΔC_{in}, in the first decimal place. Ideally, $\Delta\nu$ should be small enough so that the GIOAP model is approximately linear in the $\Delta\nu$-neighborhood about the nominal point. This is illustrated by Figure B-1 which shows how, for $y = f(x)$, $\Delta y = f(x+\Delta x) - f(x)$ differs from the approximation of Δy, $\Delta_a y$, found using the formula $\Delta_a y = f'(x)\Delta x$. In this case, if $\Delta\nu$ were much larger, the validity of using dC_{in} to approximate ΔC_{in} would be questionable. Finally, in this case, $\partial C_{in}/\partial\nu$ is negative, which means that a decrease (increase) in ν results in an increase (decrease) in C_{in}. This is intuitively plausible; however, due to the complexity of $\partial C_{in}/\partial\nu$, it is not possible to say that this is always the case.

TABLE B-4. ERRORS IN C_{in} DUE TO ERRORS IN ν

House: Baltimore Conventional (Visit #1)
Pollutant: CO

Hour	$\Delta\nu$ (air exchanges/h)	$\frac{\partial C_{in}}{\partial \nu}$ (ppm/air exchanges/h)	$\frac{\partial C_{in}}{\partial C_{in_0}}$	dC_{in}* (ppm)	ΔC_{in} (ppm)
8	-	-	-	-	-
9	-0.20	-0.3608	-	0.0722	0.07
10	-0.20	-0.5827	0.3012	0.1382	0.16
11	-0.20	-0.3132	0.3012	0.1043	0.13
12	-0.20	-0.3277	0.3012	0.0969	0.11
13	-0.20	-0.5344	0.3012	0.1361	0.16
14	-0.20	-0.5884	0.3012	0.1587	0.18
15	-0.20	-0.3042	0.3012	0.1086	0.14

* In these tables, dC_{in} (Col. 5) was computed using the following formula

$$dC_i = \underbrace{\frac{\partial C_i}{\partial C_{i-1}}}_{\text{Col. 4}} \underbrace{dC_{i-1}}_{\text{Col. 5}} + \underbrace{\frac{\partial C_i}{\partial \nu_i}}_{\text{Col. 3}} \underbrace{d\nu_i}_{\text{Col. 2}}, \quad i = 9, \ldots, 15$$

This formula is an equivalent form of equation (A-8) (see Appendix A). Also, it should be noted that any attempt to calculate dC_{in} from its components appears to result in an error. Actually, some of the values were obtained via computer and were rounded off when entered in the table.

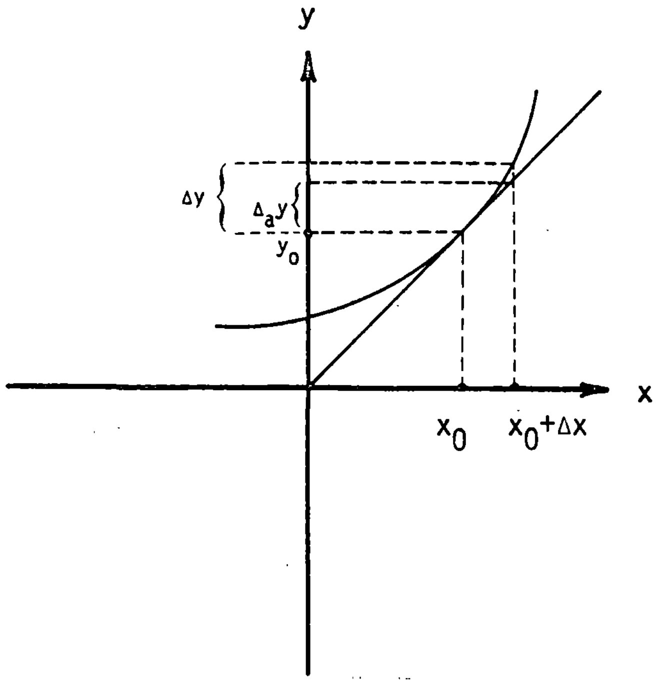

Figure B-1. Graph showing how Δy differs from $\Delta_a y$ (the approximation to Δy computed as $\Delta_a y = f'(x_0)\Delta x$).

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

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16. ABSTRACT

This report documents the formulation of the GEOMET Indoor-Outdoor Air Pollution (GIOAP) model. The model estimates indoor air pollutant concentrations as a function of outdoor pollutant levels, indoor pollutant generation sources rates, pollutant chemical decay rates, and air exchange rates. Topics discussed include basic principles, model formulation, parameter estimation, model statistical validation, and model sensitivity to perturbations of the input parameters.

The numerical estimates obtained from the GIOAP simulations have been validated with observed hourly pollutant concentrations obtained from an 18-mo residential air quality sampling program. Statistically, the model values of carbon monoxide are within 10% of the observed values in the concentration range interval which includes 85% of all hourly measurements; similarly, for nitric oxide the predicted values are within 15% of the observed; for nitrogen dioxide the difference between the predicted value and the ideal condition of exactly estimating the corresponding observed value is 16% for 85% of the observed hourly concentrations. Also, the GIOAP model predicts within 25% for nonmethane hydrocarbons and within 8% for carbon dioxide. Thus statistically the GIOAP model estimations are within 25% of the ideal condition (estimated and observed values coincide) for 85% of the observed values for CO, NO, NO_2, NMHC, and CO_2. The model has not been validated against sulfur dioxide owing to the very low values measured both indoors and outdoors. The predetermined validation criteria were not satisfied by the ozone model estimations; however, the calculated values were judged adequate because for about 85% of the observed values the predicted concentrations were within 2 ppb.

Sensitivity studies on the GIOAP model parameters indicate that errors in the estimation of the initial condition and the volume of the structure dissipate with time. Errors in estimating the air exchange rate, the indoor generation strength, and the indoor chemical decay rate are more significant. Sensitivity coefficients have been formulated for all input parameters.

The transient term is a unique feature of the GIOAP model; the impact of this term is substantial for stable pollutants but

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
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