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HIGHWAY AIR POLLUTION DISPERSION MODELING: PRELIMINARY EVALUATION OF THIRTEEN MODELS

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PREFACE

In response to legislation requiring that each Federal agency carefully and systematically consider the environmental effects of its actions, the Office of the Secretary of Transportation initiated the Technology for Environmental Analysis (TEA) program at the Transportation Systems Center in FY1972 to develop unified technological capabilities in air pollution assessment as part of a family of techniques and capabilities necessary to support the development in the Office of the Secretary, and in the Operating Administrations, of planning procedures related to the environmental impact of transportation systems and facilities.

One important goal of this program is to develop maintain expertise on the availability, applicability, and performance of techniques for analyzing the environmental impact of transportation-generated air pollution. The work reported here is the second in a planned series of reports to evaluate air pollution dispersion models. It concerns the testing and evaluation of 13 highway air pollution dispersion models. Subsequent evaluations will make use of new air quality data and of improved models.

The following should be acknowledged for their cooperation and assistance in providing TSC with the air quality data which were used in this study: the Federal Highway Administration, the Washington DC Department of Highways and Traffic, and Environmental Research and Technology, Inc.

The authors are indebted to Jeffrey D. Garlitz for aiding in the programming of the statistical routines, the running of the model programs, and the editing of the report; to Bertha Gilbert for typing the report; and to Michele Fossier for aiding in the report editing.

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1. INTRODUCTION

1.1 BACKGROUND

the past two years the Technology Environmental Analysis (TEA) project Transportation Systems Center (TSC) has been acquiring highway air quality data and highway air pollution dispersion models for use in a model testing program. The original intention of this program was to evaluate the performance of these models, using numerous measures of accuracy relating to various applications of the models in decision-making. The applications were constrained to the micro-scale: distances within a few hundred feet of the road; one hour average pollutant concentrations. Only the dispersion of inert gases was considered.

Because of the inadequacies discovered in the only data available to TSC at the time of this study, it proved impossible to assess the accuracy of the available models. Instead, it was decided to treat the meteorological and traffic information as a synthetic data set and to examine how closely the predictions of the models agree with one another when these data are used as input. Models that produce predictions which cluster closely together are defined as Consensus Models and an ensemble of such models is called a Consensus Cluster.

The identification of Consensus Clusters will assist both Federal and State DNT officials who are concerned with air quality. The Federal decision-maker can at least be assured that an analysis made with a Consensus Model represents a consensus of several existing models, while the State highway engineer can make a cost effective model selection from the Consensus Cluster for use in conducting an air quality analysis.

1.2 TYPES OF AIR POLLUTION DISPERSION MODELS

A dispersion model is a mathematical structure which accepts data on source emissions, meteorological conditions, geographic boundaries, etc., as inputs; computes the dispersion of pollutants by the

atmosphere; and produces output estimates of the concentration of pollutants over the area of interest for specified time periods. In a recent state-of-the-art survey of dispersion models [1], Darling notes that most of them fall into one of five categories:

- a. Gaussian models which assume that the dispersion of pollutants can be represented by a Gaussian process,
- b. Conservation of mass models which require the solution of the partial differential equations governing turbulent diffusion,
- c. Box models which assume that pollutant concentrations are homogeneous throughout a prescribed region,
- d. Statistical methods which use regression theory to develop an empirical relationship between concentrations and emissions, and
- e. Solutions of the complete Navier-Stokes equations for turbulent fluid motions.

This survey found that nearly all of the models currently being used in the air pollution field are either Gaussian or conservation of mass models. A general discussion of these two types of models, based upon the survey, may be found in section 2.

1.3 MODEL TESTING PROCEDURE

The Transportation Air Pollution Studies (TAPS) System [2] has been designed for use in testing and evaluating air pollution dispersion models. The TAPS System is a package of computer programs for storing, manipulating and retrieving air quality data. The System also contains routines for analyzing the performance of dispersion models, as well as programs to generate both tabular and graphical output. The TAPS System is fully operational and will be used to validate models as soon as adequate air quality data become available.

The model testing approach entails:

- a. The collection of air quality data for incorporation in the TAPS System. These data include emissions, meteorology, pollutant concentrations, and geography for the area of interest.
- b. The acquisition of air pollution dispersion models for testing. Where possible, models are implemented on TSC computers and tested in-house. Otherwise, air quality data are furnished to the model developer to be run at his plant. In this case the model predictions are returned to TSC for analysis.
- c. The evaluation of model performance. The predictions of each model are compared with the corresponding measured pollution values and the model's performance is evaluated by a series of statistical tests embedded in the TAPS System.
- d. The reporting of test results to DOT, EPA, and other agencies at the state, municipal, and local levels which are concerned with transportation-related air pollution. The present report is the first in a series of such test reports.
- e. The awarding of research and development contracts to those firms whose models are judged to have the greatest potential for DOT applications.

While this initial testing cycle has been restricted to highway air pollution dispersion models, it should be noted that the scope of this program is multi-modal. As suitable models and data become available, the state of the art in the analysis of air pollution from airports, railroads, harbors, etc., will be assessed.

Section 3 discusses both the TAPS System and the TSC model testing procedure in more detail.

1.4 AVAILABLE MODELS

During the past several years contact has been made with individuals, companies, non-profit research institutions, government agencies and universities in the air pollution modeling field. Through these contacts the 13 groups which participated in this model evaluation study have been identified. The models developed by these groups are currently being used in a

sizable fraction of all the highway air pollution dispersion studies being conducted in the United States, hence this collection of models adequately represents the state of the art. Of these 13 models, 6 are Gaussian, 6 are conservation of mass, and 1 is exponential, thus the models are distributed among the prevailing types.

Section 4 identifies the 13 models that were tested.

1.5 AVAILABLE DATA

Research and Technology, Inc. (ERT) in Washington DC, was the only air quality data base available to this project that was potentially suitable for use in validating highway air pollution dispersion models. The Airedale data base contains 1300 cases at 6 sites, including 2 at-grade, 2 elevated, and 2 depressed highway segments. All of these data were entered into the TAPS System. Subsequently, in selecting candidate cases for model validation, it proved necessary for various reasons to reject all but 230 cases out of the original 1300. Later, after an exhaustive statistical analysis of these 230 cases, it was discovered that even this selected small sample was not suitable for use in assessing the accuracy of the models.

Section 5 discusses the Airedale data base and explains the basis for rejecting the use of these data for assessing the accuracy of models. A methodology for testing the internal consistency of an air quality data set is discussed and it is recommended that all data samples be tested in this way prior to their use in testing models for accuracy.

1.6 CLUSTERING ANALYSIS

It was decided to shift emphasis from the assessment of model accuracy (which was not possible with the Airedale data) to model comparisons, one against another. This approach was possible because those Airedale data elements which are model input parameters (i.e. wind, atmospheric stability, and highway source strength) are physically realizable even though they have little relationship to the measured pollution. Therefore, the measured pollution values

were discarded and the model input parameters were treated as a synthetic data set. Model predictions with this data set as input were compared with one another in order to determine whether certain models could be grouped on the basis of close agreement among their predictions. Models which naturally cluster into such groups were defined as Consensus Models.

When this analysis was performed, 5 models (3 Gaussian, 2 conservation of mass) were found to be grouped in a very small cluster. The details of this analysis are presented in section 6.

2. TYPES OF AIR POLLUTION DISPERSION MODELS

As mentioned in Section 1.2, nearly all of the models currently being used in the air pollution field are either Gaussian or conservation of mass models. This Chapter discusses these two predominant types of models. (This material is taken from Reference 1.)

2.1 CLASSICAL GAUSSIAN MODELS

Gaussian techniques for modeling the dispersion of pollutants in the atmosphere are still the most widely used tools in the field. In this section the various Gaussian equations are stated; methods of solution are discussed; and the limitations of these equations are examined.

2.1.1 Gaussian Puff Model

The Gaussian Puff equation is considered first since all other Gaussian equations can be derived from it. This equation delas with the instantaneous emission of a finite puff of material from a point source at height H. The concentration, $\chi_1(x,y,z,t)$, of material is experssed by the equation:

$$\chi_{1}(x,y,z,t) = \frac{Q}{(2\pi)^{3/2} \sigma_{x} \sigma_{y} \sigma_{z}} \exp \left[-\left[\frac{(x-\overline{u}t)^{2}}{2\sigma_{x}^{2}} + \frac{y^{2}}{2\sigma_{y}^{2}} \right] \right]$$

$$\cdot \left\{ \exp \left[-\left[\frac{(z-H)^{2}}{2\sigma_{z}^{2}} \right] + \exp \left[-\left[\frac{(z+H)^{2}}{2\sigma_{z}^{2}} \right] \right] \right\} ,$$
(1)

Q, amount of material emitted (g).

x,y,z, Cartesian coordinates with positive x being the downwind direction

t, time since emission of the puff

 $\overline{\mathbf{u}}$, mean wind transporting the material

 σ_x , σ_y , σ_z , standard deviations of the material concentration distribution in the three coordinate directions relative to the puff center with origin ($\vec{u}t$, o, H)

Figure 1 shows a conceptual sketch of the Gaussian puff model. Note the Gaussian character of the component distributions of pollutant material.

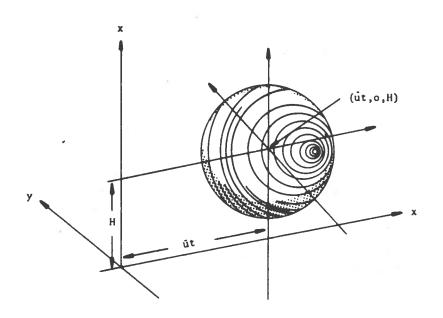
2.1.2 Gaussian Plume Model

Continuous emission from a point source may be regarded as an infinite series of puffs which spread out into a continuous plume (see Figure 2). Thus, the Gaussian Plume equation is the steady state version of the Gaussian Puff equation and is derivable by integrating Equation 1 with respect to time and keeping σ_χ constant as the puff passes any point:

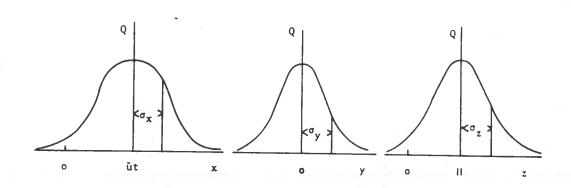
$$\chi_{2}(x,y,z) = \int_{\infty}^{\infty} \chi_{1}(x,y,z,t) dt$$

$$= \frac{Q}{2\pi\sigma_{y}\sigma_{z}\overline{u}} \exp \left[-\frac{y^{2}}{2\sigma_{y}^{2}}\right]$$

$$\cdot \left\{ \exp \left[-\frac{(z-H)^{2}}{2\sigma_{z}^{2}}\right] + \exp \left[-\frac{(z+H)^{2}}{2\sigma_{z}^{2}}\right] \right\}, \qquad (2)$$

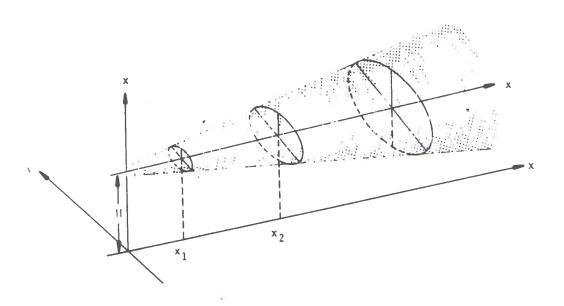


A. Three Dimensional Puff of Material

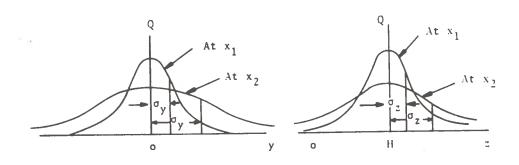


B. Component Distributions of Material about Axes through (\overline{ut}, o, H)

FIGURE 2-1. SCHEMATIC REPRESENTATION OF GAUSSIAN PUFF MODEL



A. Three Dimensional Plume of Material



B. Component Distribution of Material About (x_1,o,H) and (x_2,o,H)

FIGURE 2-2. SCHEMATIC REPRESENTATION OF GAUSSIAN PLUME MODEL

where Q is now the source emission rate of material (g/sec) x is in the downwind direction along the plume axis σ_y , σ_z are standard deviations of the material concentration distribution in the y and z directions relative to the plume axis

The Gaussian Plume equation can readily be modified to handle both linear and area sources as shown below.

2.1.3 Gaussian Line Source Models

Consider a finite line at height H extending from y_1 to y_2 , $y_1 < y_2$, perpendicular to the mean wind which blows in the x direction. The line emits at a constant rate, q, per unit length (g sec⁻¹ m⁻¹). Then

$$\chi_3(x,y,0) = \frac{2q}{\sqrt{2\pi} \sigma_z \overline{u}} \exp - \left[1/2 \left(\frac{H}{\sigma_z}\right)^2\right].$$

$$\int_{p_1}^{p_2} \frac{1}{\sqrt{2\pi}} \exp -\left(\frac{p^2}{2}\right) dp, \qquad (3)$$

where

$$p_i = \frac{y_i}{\sigma_y}$$
, $i = 1,2$

If the finite line source is on the ground, as would be the case for a road or airport runway,

$$\chi_3(x,y,0) = \frac{2q}{\sqrt{2\pi} \sigma_z u} \int_{p_1}^{p_2} \frac{1}{\sqrt{2\pi}} \exp -(\frac{p^2}{2}) dp$$
 (4)

If the line is of infinite length,

$$\chi_4(x,y,0) = \frac{2q}{\sqrt{2\pi} \sigma_z \overline{u}} \exp \left[1/2 \left(\frac{H}{\sigma_z}\right)^2\right]. \tag{5}$$

If the infinite line is on the ground, there results the simple form:

$$\chi_4(x,y,0) = \frac{2q}{\sqrt{2\pi} \sigma_z u}$$
 (6)

Finally, if the wind is blowing at an angle φ (<45°) with respect to the infinite line, Equations 5 and 6 become

$$\chi_4(x,y,0) = \frac{2q}{\sin\phi \sqrt{2\pi} \sigma_z \overline{u}} \quad \exp \left[1/2 \left(\frac{H}{\sigma_z}\right)^2\right], \quad (5a)$$

$$\chi_4(x,y,0) = \frac{2q}{\sin\phi\sqrt{2\pi}\sigma_z\overline{u}} . \qquad (6a)$$

2.1.4 The Gaussian Area Source Model

An area may be treated as a crosswind line source with a normal distribution of material, σ_y . The area source is assumed to have an initial standard deviation, σ_{yo} . The area can be treated using Equation 2 by defining a virtual upwind distance for a point source which would produce the desired σ_{yo} at the initial position of the area source. The initial vertical variation of emissions because of the distribution of source heights is represented by an initial σ_{zo} which can also be handled by defining an upwind virtual point source at the proper distance.

2.1.5 Solution of the Gaussian Equation

The Gaussian equations are receptor-oriented, which is to say that they are best suited to computing the concentrations of pollutants at specific locations because of emissions from a given source.

The principle of superposition is used to compute the concentration at a receptor of pollutants from multiple sources. If the number of source/receptor combinations is small, the problem can readily be solved using the graphs and nomograms in the reports by Taylor 30 and Beals. 31 On the other hand, large dispersion problems, involving multiple sources and many receptors, must be solved on a digital computer. If concentrations at a large number of receptors are required, the computation time can be reduced by calculating backward trajectories from each receptor and then determining the appropriate weighted contribution of all sources along that trajectory during the time period in question.

The Gaussian equations are not well suited to computing concentrations over a rectangular grid. On the other hand, the conservation of mass models to be described later are well suited for that purpose.

2.1.6 Limitations of Gaussian Models

The simplicity of the classical Gaussian models has been achieved at the expense of assumptions which restrict their application to real-world dispersion problems. Various assumptions and resulting limitations are discussed below.

It should be noted that the downwind dimension x does not appear in Equation 2 although χ_2 is a function of x,y, and z. This is because the equation is derived in such a way that both $\boldsymbol{\sigma}_{_{\boldsymbol{v}}}$ and $\boldsymbol{\sigma}_{_{\boldsymbol{\tau}}}$ are functions of x, hence the dimension x is implicit. In turn, σ_{y} and σ_{z} are functions of atmospheric turbulence, topographic characteristics, wind speed, sampling interval, and other variables. In order to solve the equation, these complex dependencies must somehow be taken into account. The standard approach has been to define a set of five atmospheric stability classes in terms of quantities which are readily observable, namely surface wind speed and incoming solar radiation for daytime situations; or surface wind and degree of cloudiness for the night. For each stability class, $\sigma_v(x)$ and $\sigma_z(x)$ have been determined empirically. These relationships obtain for a sampling interval of ten minutes, for the lower several hundred meters of the atmosphere, and over flat terrain. Their use under other

conditions, though frequently undertaken, is questionable.

The Equations 2 - 6 apply only to the continuous emission from a source, be it a point, line, or area. Also, dispersion in the downwind direction x is neglected. Therefore, the equations in their original form are not strictly applicable to many realworld problems, especially those involving transportation sources which tend to vary in both space and time. Furthermore, the equations deal only with the diffusion of stable gases or aerosols (i.e., particles of $<20\mu$ diameter) which are assumed to remain suspended in the atmosphere in the atmosphere indefinitely. Hence photochemical reactions are not considered. In addition, since mass continuity is maintained, the Gaussian equations require that no material be removed from the plume as it moves downwind (i.e. total reflection of the plume takes place at the earth's surface).

The requirement that a single mean wind \overline{u} over the entire three dimensional area of concern be introduced to transport the emitted material is contrary to the known behavior of winds. In fact, it is known that the wind generally increases with height in the lower several hundred meters of the atmosphere, hence the use of a single mean wind will tend to result in an underestimate of concentrations at lower levels and an overestimate at higher levels. Also, since \overline{u} appears in the denominator of Equations 2 - 6 it is apparent that all of these equations become unstable in the case of very light or calm winds.

Problems are posed by the existence of a temperature inversion, or stable layer, in the atmosphere which prevents the upward spread of pollutants. The region below such an inversion is called the mixing layer (since, in general, the atmosphere is completely mixed by turbulence in such a layer) and the inversion is called the mixing level. When such conditions exist, the equations are modified in such a way that the plume material distribution in the vertical becomes uniform at a certain distance downwind from the point where the plume encounters the mixing level. The distribution in the horizontal remains Gaussian.

Also, the use of the superposition principle is questionable in the case of turbulent atmospheric flow.

2.2 CONSERVATION OF MASS EQUATION

A number of investigators have adopted a more fundamental approach to the dispersion problem by attempting to solve the equations governing the conservation of pollutant mass. In the literature, work on the conservation of mass equations is described by Sklarew (5), Eschenroeder and Martinez (6), Roth et al (7) and Egan and Mahoney (8).

The general conservation equation for a particular pollutant may be written in vector form, as follows:

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot (\nabla c_i) + \nabla \cdot (D\nabla c_i) + R_i + S_i$$
(7)

with c_{i} concentration of species i

i = 1,2,3...p species

 \vec{V} , the wind velocity with components u,v, and w in the x,y, and z directions

$$\nabla = \frac{\partial}{\partial \dot{x}} \dot{i} + \frac{\partial}{\partial y} \dot{j} + \frac{\partial}{\partial z} \dot{k}$$

x, y, z, component directions

i, j, k, unit vectors in directions x, y, z, respectively

D, molecular diffusivity tensor

 $\mathbf{R}_{\mathbf{i}}$, rate of generation of species i by photochemical reactions

 $\mathbf{S}_{\mathbf{i}}$, emission source strength for species \mathbf{i} .

Equation (7) governs changes in concentration of a particular species i at a point in the atmosphere. It states that the concentration change, $\frac{\partial c_i}{\partial t}$, is equal to the net effect of four processes: (a) the advection (or transport) of pollutant, $\nabla \cdot (\vec{v} c_i)$; (b) the molecular diffusion, $\nabla \cdot (D\nabla c_i)$, of pollutant; (c) the change caused by photochemical reactions, R_i ; and (d) the emission source

strength, S_i, of the pollutant.

The concentration and the wind can be assured to

The concentration and the wind can be expressed in terms of turbulent deviations from their time-averaged values:

$$c_{i} = \overline{c}_{i} + c'_{i},$$

$$\overrightarrow{v}_{i} \cdot \overrightarrow{v}_{i} + \overrightarrow{v}'_{i},$$
thus
$$u_{i} = \overline{u}_{i} + u'_{i},$$

$$v_{i} = \overline{v}_{i} + v'_{i},$$

$$w_{i} = \overline{w}_{i} + w'_{i},$$

where bars above quantities denote time-averaged values and primes indicate turbulent eddy fluctuations.

By introducing the above expressions into Equation 7, taking time averages of each term, expanding, and rearranging terms the following equation is obtained for the conservation of mass of species i in a turbulent atmosphere:

$$\frac{\partial \overline{c_i}}{\partial t} + \frac{\partial (\overline{uc_i})}{\partial x} + \frac{\partial (\overline{vc_i})}{\partial y} + \frac{\partial (\overline{wc_i})}{\partial z} + \frac{\partial (\overline{u'c_i'})}{\partial x} + \frac{\partial (\overline{u'c_i'})}{\partial x} + \frac{\partial (\overline{v'c_i'})}{\partial y} + \frac{\partial (\overline{w'c_i'})}{\partial z}$$

$$= D_{i} \left(\frac{\partial^{2} \overline{c}_{i}}{\partial_{x}^{2}} + \frac{\partial^{2} \overline{c}_{i}}{\partial_{y}^{2}} + \frac{\partial^{2} \overline{c}_{i}}{\partial_{z}^{2}} \right) + R_{i} + S_{i}.$$
 (8)

In order to reduce Equation 8 to a form tractable for solution, the following assumptions are made:

- a.. Molecular diffusion is negligible in comparison to turbulent diffusion, hence $D_i = 0$.
- b. Atmospheric flow is incompressible, hence

$$\frac{\partial \overline{\mathbf{u}}}{\partial \mathbf{x}} + \frac{\partial \overline{\mathbf{v}}}{\partial \mathbf{v}} + \frac{\partial \overline{\mathbf{w}}}{\partial \mathbf{z}} = 0.$$

c. The turbulent eddy diffusion coefficients K_x , K_y , K_z may be defined as follows:

$$\overline{u^{\dagger}c_{i}^{\dagger}} = -K_{x} \frac{\partial \overline{c}_{i}}{\partial x} ,$$

$$\overline{v^{\dagger}c_{i}^{\dagger}} = -K_{y} \frac{\partial \overline{c}_{i}}{\partial x} , \text{ and}$$

$$\overline{w^{\dagger}c_{i}^{\dagger}} = -K_{z} \frac{\partial c_{i}}{\partial z} . _{2-10}$$

Introducing these assumptions into Equation 8:

$$\frac{\partial \overline{c}_{\mathbf{i}}}{\partial \mathbf{t}} \leftarrow \overline{u} \frac{\partial \overline{c}_{\mathbf{i}}}{\partial x} \leftarrow \overline{v} \frac{\partial \overline{c}_{\mathbf{i}}}{\partial y} + \overline{w} \frac{\partial \overline{c}_{\mathbf{i}}}{\partial z} = \frac{\partial}{\partial x} \left(K_{\mathbf{x}} \frac{\partial \overline{c}_{\mathbf{i}}}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{\mathbf{y}} \frac{\partial \overline{c}_{\mathbf{i}}}{\partial y^{-}} \right) +$$

$$\frac{\partial}{\partial z} \left(K_z \frac{\partial \overline{c_i}}{\partial z} \right) + R_i + R_i . \tag{9}$$

Even further simplification can be achieved by introducing the following additional assumptions:

- The horizontal wind field is a uniform flow in the x-direction,
- b. The vertical velocity component $\overline{\boldsymbol{w}}$ can be neglected, and
- c. Horizontal eddy diffusion can be neglected.

With these assumptions Equation 9 reduces to:

$$\frac{\partial \overline{c}_{i}}{\partial t} + \overline{u} \frac{\partial \overline{c}_{i}}{\partial x} = \frac{\partial}{\partial z} \left(K_{z} \frac{\partial \overline{c}_{i}}{\partial z} \right) + R_{i} + S_{i} . \quad (10)$$

A salient feature of these equations is that they represent conditions over a three-dimensional grid and hence do not require the source-receptor formulation of the Gaussian equations. Instead, all sources enter cells of the grid and all concentrations are computed for those same cells. Thus, the model is spatially-oriented which greatly simplifies computations for a large number

of sources since each additional source affects only a single cell (or at most a few cells).*

2.2.1 Solution of Conservation of Mass Equations

There are two basic approaches to solving these equations: the fixed coordinate or Eulerian method, and the moving cell or Lagrangian method. In the Eulerian method, the air space is subdivided into a fixed three-dimensional grid with cells a few miles on a side in the horizontal and a few hundred feet in the vertical. The solution is obtained for each cell in this fixed grid at short intervals of time. In the Lagrangian method, columns of air are advected through the air space and solutions are obtained within the moving columns. There are many mathematical subtleties in both the Eulerian and Lagrangian solutions to these equations. Detailed discussions of this subject can be found in any of the four references at the beginning of this section. Application of these equations has only recently been undertaken, in contrast to the long history of Gaussian solutions.

2.2.2 Aspects of Conservation of Mass Equations

It is instructive to examine the aspects of these equations which differentiate them from the Gaussian formulations. First, $\sigma_y(x)$ and $\sigma_z(x)$ are replaced by the diffusion coefficients K_x , K_y and K_z . Although the dependence on stability has been eliminated, the problem of estimating the diffusion coefficients remains. There is no completely satisfactory way of doing this. Some investigators appeal to theory, others rely on empirical methods, and still others attempt to compute these coefficients from the data.

The conservation of mass equations, because of their cellular structure, are able to accommodate variable emission rates.

It should be noted that Donaldson and Hilst²³ use a somewhat different approach. Their equation is based upon the complete Navier-Stokes equations for turbulent fluid motions and includes terms describing the turbulent flux of pollutants. This is an even more general method than the simple conservation of mass approximation, but solution of the complete equations is a formidable computing task.

Typically, the assumption is made that emissions remain constant over a period of one hour or so. Furthermore, through the $R_{\rm i}$ terms, the equations handle photochemical reactions directly. The functional form and number of these reactions are at the discretion of the modeler and empirical data on the character and speed of such reactions can readily be incorporated in the model.

Another advantage of the grid structure is that a separate wind can be entered for each cell. (How such a three-dimensional distribution of winds is obtained is a subject for another section.) The wind field can be updated at every time step if the data are available. Also, the existence of a stable layer in the atmosphere poses no problem for the conservation of mass model. The mixing level can simply be defined as an impervious boundary condition (i.e., $K_Z=0$). A change in the mixing level is handled in the same way at the appropriate time step.

In summary, then, it is clear that the conservation of mass model overcomes many of the limitations of the Gaussian models and hence is potentially a more powerful tool for analyzing air pollution problems.

3. MODEL TESTING PROCEDURE

3.1 PROCEDURE

The model testing approach consists of three basic steps:

- a. The collection of air quality data for incorporation in in the TAPS System,
 - b. The running of models to obtain test outputs
 - c. The evaluation of model performance

The foundation of any model validation study is a large sample of good highway air quality data. (However, very little air quality data of this type are currently available.) These should include emissions, meteorological and background data, as well as a complete site description. In the future, several samples of this type of data for a number of different roadway configurations are expected to become available.

3.2 TRANSPORTATION AIR POLLUTION STUDIES (TAPS) SYSTEM

The Transportation Air Pollution Studies (TAPS) System [2] is a set of computer routines which allows transportation—source air pollution data to be stored in the TAPS Data Base and then used to validate and evaluate transportation—source air pollution dispersion models. Specifically, the TAPS System allows (1) data to be stored in the TAPS Data Base, and retrieved from it, (2) dispersion model programs to be run using the retrieved data as input, and (3) the resulting output of the model program to be compared with measured values and with the results of other model programs to produce an evaluation of the model.

3.2.1 System Description

The TAPS System consists of four parts: (a) FORMAN (the FORmat MANipulator), (b) DARES (the DAta REtrieval System), (c) SMOG (the Standard Model Output Generator), and (d) DIMOTE (the DIspersion Model TEst). Briefly, FORMAN stores incoming data in the TAPS Data Base; DARES retrieves data from the TAPS Data Base in a form acceptable as input to the model program being evaluated; SMOG transforms the model program's output to a standard form; and DIMOTE evaluates the model, using a variety of statistical tests to compare the program's output with the results obtained by other model programs and also with the measured values.

The use of TAPS System is illustrated in Figure 3-1. Its operation is as follows:

a. Incoming Data-Set

For each new transportation-source air pollution data-set received:

- 1) A set of FORMAN commands is written.
- 2) The FORMAN Processor uses the FORMAN commands and the new data set as input, and inserts the data set into the TAPS Data Base in standard form.

b. Incoming Model Programs

For each new transportation-source air pollution dispersion model program received, a set of DARES commands is written corresponding to the program's inputs.

c. Model Testing.

To test a given model program using a selected data set from the TAPS Data Base:

- 1) The DARES Processor is run using the model's DARES commands as input. It retrieves from the TAPS Data Base a set of test data (from the selected data set) which is in the proper form for input to the model program.
- $\,$ 2) The model is run using the test data produced by the DARES Processor as input.
- 3) SMOG converts the model program's output to a standard output form.
- 4) Selected DIMOTE Routines are run using the standard output produced by SMOG as input. DIMOTE compares the tested model's output with the values that were measured and with the outputs previously produced by other models for the same input data set. A variety of statistical tests are employed.
- 5) Based on the results of the statistical tests, DIMOTE produces a set of graphs and tables which provide an evaluation of the model and a comparison with other models.

3.2.2 System Implementation

The TAPS Data Base is disk-oriented, and thus a third-generation computer system should be used for the implementation of the TAPS System programs. Since most models to be tested were written in FORTRAN IV for the IBM 360 or 370 computers, it was decided to implement the TAPS System on an IBM 360/75, using FORTRAN IV. This allows the power of disk storage to be used by TAPS and also keeps to a minimum the task of converting models from one computer system to another.

The individual TAPS components are discussed in detail below.

3.2.3 FORMAN

The element of the TAPS System that deals with incoming data is the FORmat MANipulator, FORMAN. FORMAN's function is to take any data set which has been acquired by the Transportation Systems Center, convert it into TAPS Standard Format, and store it in the TAPS Data Base.

The Center expects to receive highway and airport air pollution data sets from many sources. In most cases the data sets were originally acquired for use in other projects and therefore are received in various formats which are tailored to the original application. Also, various media may be used to transmit the data to TSC; e.g., punchcards, magnetic tape, computer printouts, or even handwritten lists. FORMAN allows the user to extract conveniently the data set from the medium in which it is received (in whatever format it is received) and store it in TAPS Standard Format in the Data Base. The process of converting the data set from an arbitrary input form to the TAPS Standard Format is accomplished by the FORMAN Processor. A set of FORMAN Commands is written for each incoming data set which describes the format of the data set in terms of the TAPS Standard Format. This set of commands is input to the FORMAN Processor along with the data set. The FORMAN Processor reads the Commands and enters the data set into the TAPS Data Base in TAPS Standard Format as directed by the Commands.

3.2.4 <u>DARES</u>

Data are retrieved from the TAPS Data Base by the DAta REtrieval System, DARES. The function of DARES is to retrieve the data of an air pollution data set chosen from the Data Base and to prepare these data in a format which can be directly accepted as input by the given air pollution dispersion model being tested.

In general, since each model program will be tested using several of the data sets stored in the TAPS Data Base, a method is needed to allow a model to be run using as input the data of any given data set in the Data Base. Two alternative methods can be considered. The first would be to change each model's input commands so that the model program could read directly from the TAPS Data Base. The second would be to retrieve the data from the TAPS Data Base and construct, prior to the running of the model, a set of card images in the input format expected by the model program. This latter alternative was chosen for DARES for three reasons: (1) it is desirable to alter the model program being tested as little as possible, (2) a more accurate evaluation of the computer time used by the model can be found if all input retrievals are performed prior to model run, and (3) error conditions resulting from the lack of a match between the data requirements of the model and the data stored in the chosen data set can be more easily handled utilizing software fixes or error message printouts.

The process of retrieving desired data from a chosen data set in the TAPS Data Base and forming them into card images acceptable to the tested model program is accomplished by the DARES Processor. For each model program to be tested, a set of DARES Commands is written describing the expected input cards to the program. The DARES Commands describe the data which must be retrieved from the TAPS Data Base in terms of the standard position where such data are stored in the Data Base. In addition, the Commands indicate the position where such data should be placed on a card image and what other information should be included to form the card image in the format the program expects.

3.2.5 SMOG

The part of the TAPS System which deals with model outputs is the Standard Model Output Generator, SMOG. SMOG consists of a set of routines which are used to convert each model's output from its usual form to a standard form and then place it in the TAPS Data Base. The model outputs are then used as input to the DIMOTE test package.

3.2.6 DIMOTE

The fourth and final part of the Transportation Air Pollution Studies Systems is the DIspersion MOdel TEst, DIMOTE. DIMOTE's function is to take the outputs of the model program runs (which have been stored in the TAPS Data Base by SMOG) and compare them

with each other and with the measured values (which were stored with the other incoming data for each site and case by FORMAN). DIMOTE uses several statistical tests (see Appendix E) for these comparisons, and then produces tables and graphs comparing and evaluating the different model programs. These results are used in the production of reports on model program evaluation.

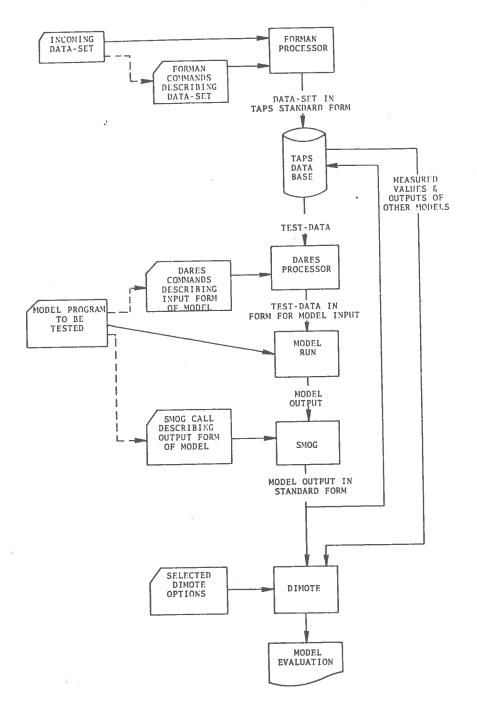


Figure 3-1 Transportation Air Pollution Studies System

4. AVAILABLE MODELS

4-1 REQUEST FUR COMPANY PARTICIPATION

In February of 1974, an exploratory letter was sent (Appendix A) to several companies who had previously expressed an interest in participating in dispersion model validation experiments. These companies were among those which had responded to an earlier questionnaire sent to model developers in the course of preparing a state-of-the-art survey on computer modeling of transportation-generated air pollution [1]. In this letter, the purpose of these experiments was explained, the types of input data to be furnished were specified, and the desired output format was defined.

4-2 PARTICIPATING COMPANIES

response to this exploratory letter, 10 agreed to participate in this initial companies experiment either by supplying a copy of their dispersion model for in-house testing, or by running their model under contract in their own plant using data supplied to them. (Appendix B contains the letter accompanying the data sent to the eight companies participating under contract.) These models, together with three dispersion models already available in-house, brought the total number of dispersion models to be tested in this experiment to 13. Appendix C contains descriptions (provided by the individual companies) of these 13 models.

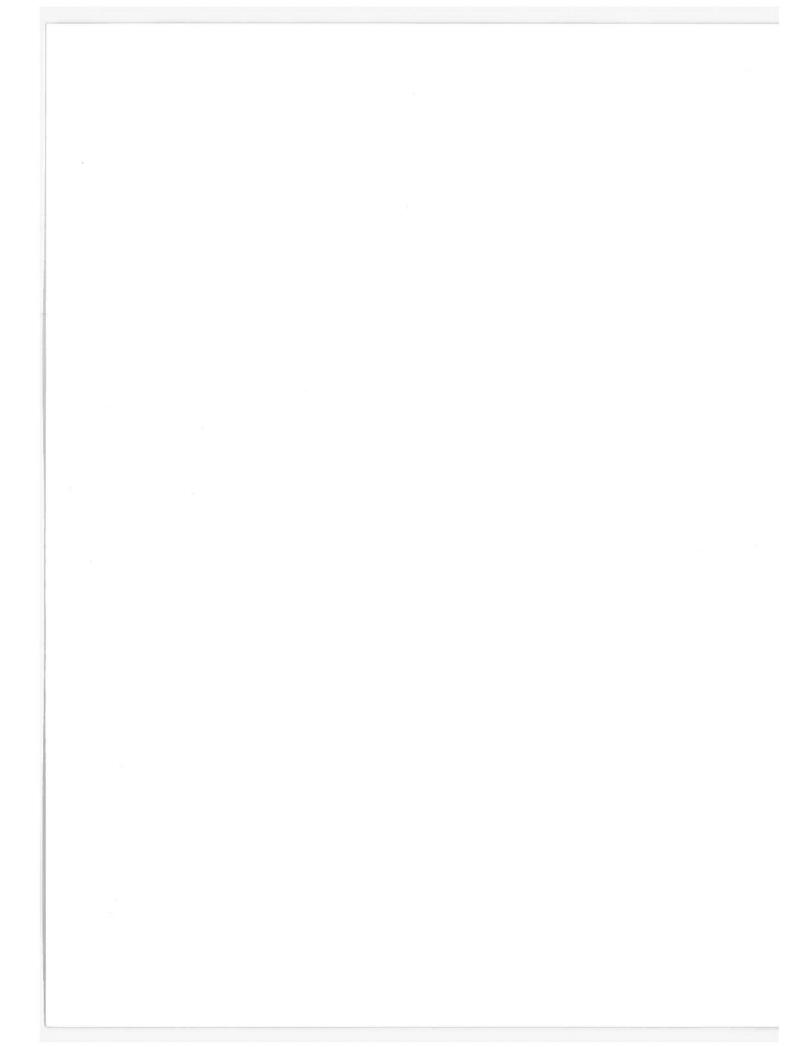
Table 4-1 shows the type of model, the testing mode (in-house or contract), and the sites for which the model was run for each participating company. The company codes shown in the second column of this table will be used in section 6 in discussing the results of the clustering analysis. Company comments on various aspects of this study can be found in Appendix D.

The models of two participating companies, Fnvironmental Research and Technology, Inc. (ERT) and the Center for the Environment and Man (CEM), were not tested on Site 11 data. ERT used a 12-ft center strip while other participating companies used a 95-ft center strip. This discrepancy is discussed in the ERT comments in Appendix D and also in Appendix F. Because

TABLE 4-1. STUDY PARTICIPANTS

						-	Sites fo	for Which
			Model Type		Testing Mode	Mode	Model was Run	as Run
					1-		Independence	Military
			Conservation				Avenue,	Road,
COMPANY/AGENCY	CODE	Gaussian	of Mass	Other	Contract	Other Contract In-House	Site 11	Site 14
AeroVironment	AER		×		×		×	×
California Division of Highways	CAL	×				×	×	×
Center for the Environment & Man	CEM		×		×			×
Environmental Research & Technology	ERT		×		×			×
Environmental Systems Laboratory	ESL	×				×	×	×
General Electric	89			×		×	×	×
	TNT		×		×		X	×
Vamen Sciences Cornoration	KAM	×			×		X	×
Lockheed Missiles and Space	LOC		×		×		X	×
Systems Control. Inc.	SCI	×			×		×	×
System. Science and Software	SSS		×		×		×	×
TSC/EPA	TSC	×				×	×	×
Walden Research, Inc.	WAL	X				×	×	×

of time constraints CEM results for this site could not be included in the testing.



5. AIREDALE DATA

5.1 DATA SELECTION

The Airedale data set used in this study was collected as part of Contract No. HT-7202 with the Department of Highways and Traffic, Government of the District of Columbia, Office of Planning and Programming. This program was sponsored jointly by the Department of Highways and Traffic, and the Federal Highway Administration.

In selecting cases suitable for model validation, TSC rejected 1059 cases. The data from one elevated and two depressed sites were rejected because of the presence of extraneous nearby pollution sources, which would mask the pollution resulting from the highway of interest.

At the three sites chosen by TSC for its model validation study, a total of 674 cases were available for use. Upon inspection of these data it was determined that a majority of the cases were not suitable for utilization in the study. Some cases were suspect because of very low or very high wind speed; other cases were found that had very light traffic counts. Also, a large number of cases were found in which the measured upwind pollution at one or more receptors exceeded the measured pollution at the corresponding downwind receptor, due to either a measurement error or the influence of a source upwind of the roadway.

TSC used the following criteria in an attempt select representative cases for this study: (1) carbon monoxide reading for a downwind receptor must be greater than the corresponding upwind receptor reading. (2) In general, very light traffic cases were omitted. (However, a few of these cases were included as test data to determine how well dispersion models could handle them.) (3) Only cases with wind speeds greater than one meter per second were used. (4) It was desirable, from a dispersion model point of view, to include only test cases in which the angle of the wind with the road exceeded 12.5 degrees. In reality, these conditions do occur and thus several such cases were included as part of the data for Site 11, Independence Avenue. However, the test data for Site 14, Military Road, contain no case where the angle of the wind to the road is less than 20 degrees.

It was found that only 230 cases met the above four criteria, 150 at Independence Avenue and 80 at Military Road. This was the candidate data set for use in the proposed model validation experiments.

5.2 STATISTICAL TESTING

This reduced Airedale data set was used as input to all of the highway air pollution dispersion models following the procedure discussed in section 3. Five models were run in-house and the remaining eight were run by the participating companies under contract. Appendix G contains the measured air pollution and the predictions of all the models for these 230 cases.

During the time when the models were being run, further study of the data led to a questioning of the suitability of even the reduced data set for model validation. To resolve this issue, a series of statistical tests were performed on the reduced Airedale data set.

First, a series of rank correlation tests were run, correlating the measured pollution (background removed) with certain of the input parameters. In general, these tests showed low correlations. Next, a series of multiple regression analyses were undertaken to determine the dependence of the measured pollution (background removed) on the various input parameters.

A multiple regression analysis finds the linear combination of input parameters which best fits (in the least-squares sense) the measured pollution values. In this case it was used to find the best values for the linear coefficients A,R,C, and D in the equation:

 $M^* = Au + B |\cos\theta| + Cs + Dq$

where:

M" = the best estimate of M,

M = the measured pollution because of the highway (as estimated by the difference between the sum of the downwind pollution measurements and the sum of the upwind pollution measurements at three heights: 3, 15, and 30 feet, on towers 36 or 49 feet from the highway),

u = the wind speed,

 θ = the wind angle,

s = the stability, and

q = the source strength (found from the number of vehicles per hour and their speed, using tables from Reference 11).

The linear coefficients that are found are "best" in the sense of minimizing the square error or unexplained sum of the squares, US, as defined by:

$$US = \sum_{p=1}^{N} [M(p)-M^{*}(p)],$$

for all measurement points, p. When this is found, it is compared with the total sum of the squared deviations from the mean, TS, as defined by:

$$TS = \sum_{p=1}^{N} EM(p) - MAV(p)$$

where MAV is the average value of M:

$$MAV = (1/N) \sum_{p=1}^{N} M(p) .$$

The explained sum of the squares, ES, is defined to be:

ES = TS-US .

Then, the multiple regression coefficient, R_r is defined by:

$$R = (ES/TS)^{1/2}$$

Thus, R indicates the percentage of the total variation accounted for by the regression. R=0 indicates no linear relation between the measured pollution and the input parameters, R=1 means a perfect

linear fit, and R=0.5 means that 25% of the variation in the pollution is explained by a linear combination of the input parameters. Thus, a low value of R reflects a lack of predictability of the measured pollution from the input parameters, thereby indicating that the data are unsuitable for model validation.

A multiple regression analysis was performed for the data of Sites 11 and 14. The results are shown in Table 5-1. These results tend to confirm the doubts about the appropriateness of the data for model validation.

The relationship of the input variables to the pollution is not necessarily linear and, in fact, it can be argued that the pollution may be a multiplicative function of u, " $\cos\theta$ ", q, and SIGZ, where SIGZ, the vertical dispersion coefficient, is a function of stability and downwind distance. (This is the Gaussian formulation.) Therefore, a multiple regression analysis was run for the data of Sites 11 and 14 using:

In $M'' = A \ln u + B \ln |\cos \theta| + C \ln q + D \ln SIGZ$.

The results of these runs, shown in Table 5-2, are not significantly different from those in Table 5-1.

The final tests performed on the reduced Airedale data set was a set of clustering tests in which the data were compared against the predictions of all of the models. As will be shown in section 6, these tests provided further evidence that the data set was unsuitable for model validation.

There are many factors that might have contributed to the poor performance of the data in all statistical tests. The tests do not indicate the causes of the data problems, but these may include inadequacy of site location, inaccuracy of measurements, and inapplicability of assumptions.

On the basis of the results of the statistical tests discussed in this section, it was decided that the reduced Airedale data set could not be used to assess the accuracy of predictions. Thus, since this was the only available data set, no assessment of model accuracy could be performed in this test cycle.

As a consequence of the above findings we recommend that air quality data be statistically tested for internal consistency, by methods similar to the above, prior to their use in model testing. If the results are unsatisfactory, as in this case, then the data should not be used for assessing model accuracy.

The next section discusses an approach which treats the Airedale data as a synthetic data set which can be used to compare model predictions, one against another.

Table 5-1 MULTIPLE REGRESSION TEST 1

MULTIPLE REGRESSION

 M^{\bullet} VS. u, $|\cos\theta|$, s, and q

	Site 11	Site 14
P	0.48	0.61
Variation Explained	23%	37%

Table 5-2 MULTIPLE REGRESSION TEST 2

MULTIPLE REGRESSION In M' VS. In u, In |cos9|, In s, and In q

	Site 11	Site 14
Ŗ	9.41	0.59
Variation Explained	17%	35%

6. CLUSTERING ANALYSIS

The question arose as to whether any useful analysis could be performed on the predictions of 13 dispersion models for the reduced Airedale data set from Independence Avenue (150 cases) and Military Road (80 cases). Although it had been demonstrated (section 5) that there was little relationship in these data between the measured pollutant concentrations and the input parameters (i.e., wind, atmospheric stability, and highway source strength), nonetheless the set of input parameters themselves, are physically realizable (see Table 6-13). It was therefore decided to discard the measured pollution data and to treat the input parameters as a synthetic data set, thereby shifting the focus to model comparisons, one against The purpose of comparing models in this way another. is to determine whether the predictions of certain models tend to agree closely with each other (i.e., cluster together).

6.1 CLUSTERING

The concept of the Consensus Cluster has immediate application to air quality analysis and associated decision-making. Federal DOT officials must often rely predictions generated by models when making decisions on the environmental impact of transportation systems. If a model in the Consensus Cluster has been used for a particular analysis then the approving Federal official can at least be assured that the analysis probably represents a consensus of several existing models. Similarly, at the state level, highway are often confronted with the task of engineers selecting suitable models for use in computing the air quality impact of proposed highways. Several such models are in the public domain, while others are the property of companies which perform air quality analyses for a fee. Models will differ in the cost of running them (i.e., computations) and in the amount οf state manpower resources that must be allocated to project, and thus the cost of using the various models may vary widely. Therefore, information about which models produce similar predictions could result considerable cost savings in selecting a model for particular application. Furthermore, if the adequacy of an air quality analysis should be challenged in a court case, the state DOT involved in the suit would be in a somewhat stronger position to defend its analysis if the model used had been selected from a group which had previously been demonstrated to produce similar predictions.

In the absence of air quality data suitable for testing the accuracy of models, it is impossible to determine whether the predictions of models in a Consensus Cluster are any more accurate than the predictions of models not in the Cluster. Nonetheless, since models within a Consensus Cluster produce results which agree closely with one another, these models are not likely to harbor theoretical or programming errors in their construction.

Figure 6-1 shows a scatter diagram of the predictions of the AeroVironment and Walden Research models. Note that these two models agree very closely. Figure 6-2 is a similar diagram for the AeroVironment and G.L. models in which it can be seen that the predictions differ markedly. Models which form a Consensus Cluster would be expected to produce predictions which closely agree as in figure 6-1, whereas Figure 6-2 is an extreme example of two models whose predictions do not cluster.

6.2 DEFINITIONS

By a pairwise comparison of the predictions of two models for the same set of data points, a measure of the "distance" between their predictions can be determined. A "model cluster" can then be defined as a set of models whose predictions are less than a distance, d, apart. (The distance, d, is called the "cluster diameter," and can be defined as some fraction of the average model prediction.) If there is a single predominant cluster, then that will be called the Consensus Cluster, and all models in the cluster will be called Consensus Models.

6.3 DISTANCE MEASURES

Three types of pairwise model distance measures were used:

a. Average Absolute Difference (AAD),

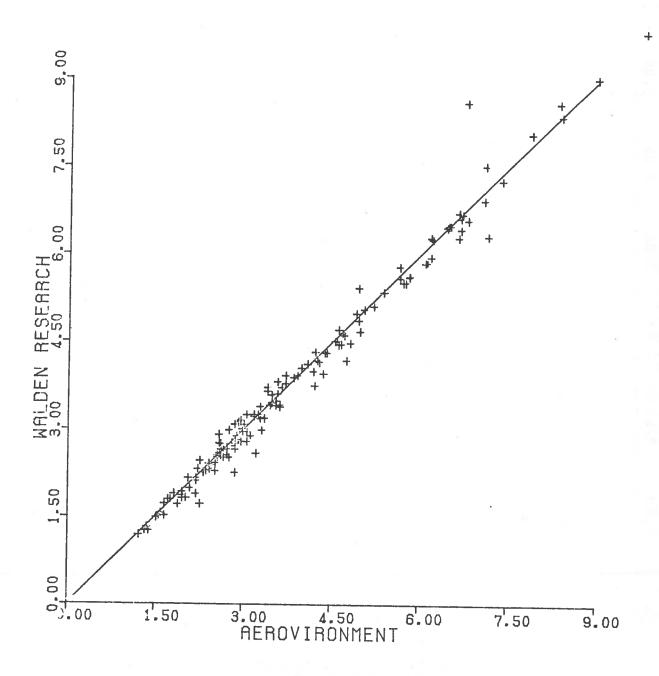


FIGURE 6-1. SCATTER DIAGRAM OF PREDICTIONS OF AEROVIRONMENT AND WALDEN RESEARCH MODELS

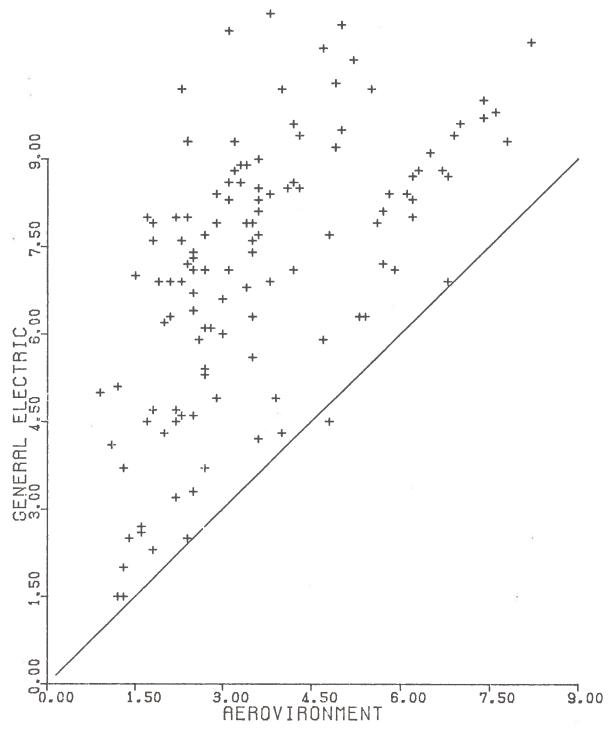


FIGURE 6-2. SCATTER DIAGRAM OF PREDICTIONS OF AEROVIRONMENT AND GENERAL ELECTRIC MODELS

- b. 80th Percentile Difference (80%D), and
- c. Correlation Coefficient (CC).

The Average Absolute Difference for two models, M1 and M2, can be found by:

AAD =
$$(1/N)$$
 $\sum_{p=1}^{N} |M1(p)-M2(p)|$,

where N is the number of points.

Two models can have a low AAD and still have large differences for many data points. Therefore, a second measure, the 80th Percentile Absolute Difference, is used. This is found by ordering all of the absolute differences, |M1(p)-M2(p)|, and finding the one that is greater than or equal to 80% of these differences.

The correlation coefficient measures the tendency of the predictions of two models to vary linearly. Thus a high correlation coefficient indicates a strong linear relationship between two models, even though there may be considerable absolute difference between their predictions. The correlation coefficient for the pollution predictions (background removed) of two models, M1 and M2, is defined as follows:

$$CC = (1/N)^{\frac{N}{\Sigma}} E(M1(p)-M1AV)(M2(p)-M2AV) \frac{1}{2} (VAR1)(VAR2),$$

$$p=1$$

where:

M1AV =
$$(1/N)^{\frac{N}{\Sigma}} M1(p)$$
,
p=1

M2AV =
$$(1/N)^{\frac{N}{\Sigma}} M2(p)$$
,

VAR1 =
$$(1/N)^{\frac{N}{\Sigma}} (M1(p)-M1AV)^{\frac{2}{N}}$$
, and

 $VAR2 = (1/N) \sum_{p=1}^{N} (M2(p)-M2AV)$.

6.4 PESULTS

For each model, M, the predicted concentration, M(p), for each data point, p, of the reduced Airedale data set was found. As discussed in section 4, 11 of the 13 models were run for Site 11 data, and all 13 models were run for Site 14 data.

Using the outputs of the model runs for models, difference matrices were found showing the AAD and the 80%D for all pairs of models for both sites 11 and 14. These are shown in Tables 6-1 and 6-2. the correlation coefficient of model matrix of predictions appears in Table 6-3. (Company names corresponding to the model coded names appearing in these and subsequent tables are shown in Table 4.1) In these three tables the far right-hand column, labeled DAT, pertains to the measured data downwind of the roadway. It can be seen that, by all three distance measures, the data are far removed from the predictions of all the models, which confirms our contention that these data are not suitable for model validation.

To determine a reasonable cluster diameter distance, the average prediction of all models for all cases was calculated. The difference between the average prediction and the average background is the average predicted pollution contribution of the roadway (which was found to be about 1ppm). The cluster diameter was then defined in terms of the average prediction. Five clusters were formed with diameters of 0.2, 0.4, 0.6, and 0.8 (i.e., 20, 40, 60, and 80% of the average prediction), thereby yielding a series of expanding Consensus Clusters. In the case of the correlation coefficient, two clustering criteria were adopted; 0.75 and 0.65.

The clusters formed by the above criteria for each site are shown in the following tables: Mean Absolute Difference clusters, Table 6-4; 80th Percentile Difference clusters, Table 6-5; Correlation Coefficient clusters, Table 6-6. For each site and criterion the

TABLE 6-1. MATRIX OF MEAN ABSOLUTE DIFFERENCE BETWEEN MODEL PREDICTIONS

Mean Absolute Difference (ppm)

		DAT	1.66 1.88 1.72 1.72 1.72 1.73 1.73 1.73 1.73 1.74 1.58
		WAL	0.37 0.08 3.08 3.08 3.25 3.25 0.50 0.50 0.50 0.50 0.50 0.50
	DAT 2.11 2.15 2.15 2.74 2.68 2.18 1.97 1.97 1.99 2.10	TSC	0.23 0.24 0.24 0.26 0.30 0.30 0.52 0.71 0.69 0.04 1.72
	WAL 0.20 0.13 0.97 3.98 1.71 0.62 0.55 0.05 0.05 0.27 0.28 0.28 0.28	SSS	0.41 0.59 3.23 0.57 0.87 2.98 0.57 0.70 0.70 0.42 0.42
	TSC 0.29 0.29 0.80 3.80 1.67 0.61 0.61 0.91 0.35 0.0	SCI	0.71 0.68 3.08 0.87 1.17 2.64 0.80 0.69 0.69 0.07 0.77 0.05
	SSS 0.30 0.34 0.91 5.96 1.75 0.72 0.65 1.04 0.0	TOC	0.67 0.52 3.48 0.96 1.29 3.04 0.91 0.75 0.0 0.70 0.71
	SCI 0.98 1.02 1.42 3.11 1.89 1.17 0.0 0.0 1.04 0.99 1.49	KVM	0.60 0.46 5.62 0.68 0.90 3.20 0.53 0.0 0.75 0.69 0.75 0.69
	LOC 0.59 0.59 1.35 3.69 1.93 1.01 0.0 0.86 0.65 0.65	INT	0.41 0.50 3.32 0.22 0.47 2.92 0.0 0.53 0.51 0.57
MODELS	KAM 0.61 0.59 0.75 3.84 1.66 0.0 1.01 1.17 0.72 0.62 2.18	GE	2.98 3.25 1.78 2.87 0.0 2.92 3.20 3.04 2.64 2.98 3.02 3.02 3.02
M	1.06 1.56 1.70 1.84 4.11 0.0 1.66 1.93 1.89 1.75 1.75	ESL	0.70 0.77 3.11 0.55 0.0 2.87 0.90 1.29 1.17 0.87 0.59
	GE 3.95 4.00 3.62 0.0 4.11 3.84 3.69 3.69 3.11 3.11 3.11 3.11 3.11 3.96	ERT	0.39 0.46 3.26 0.0 0.35 0.22 0.68 0.96 0.96 0.57
	ESL 0.92 0.87 0.0 3.62 1.84 0.75 1.35 1.42 0.91 0.97 2.15	CEM	3.37 5.68 5.00 5.11 1.78 3.32 3.62 3.62 3.43 3.43 3.43 3.43 3.43 3.43 3.43 3.4
	CAL 0.24 0.07 0.87 4.00 1.70 0.59 0.59 0.34 0.34	CAL	0.36 0.00 3.68 0.77 3.25 0.50 0.50 0.52 0.53 0.53
	AER 0.0 0.24 0.92 3.95 1.66 0.61 0.59 0.98 0.20 0.20	AER	0.0 0.36 3.37 0.39 0.70 2.98 0.41 0.67 0.67 0.71 0.41
	AER CAL CAL ESL GE INT KAM LOC SCI SCI SSS TSC WAL		AER CAL CEM ERT ESL GE INT KAM LOC SCI SSS TSC WAL DAT
	Independence Avenue, Site 11		Military Road, Site 14

TABLE 6-2 MATRIX OF 80TH PERCENTILE DIFFERENCE BETWEEN MODEL PREDICTIONS

80th Percentile Difference (ppm)

MODELS

1	DAT	3.40	3.40	3.50	4.20	4.20	3.40	3.10	2.40	3.40	3.20	3.40	0.0
	WAL	0.30	0.20	1.60	5.80	2.70	0.80	0.70	1.20	0.20	0.40	0.0	3.40
	TSC	0.40	0.40	1.30	5.60	2.70	0.80	06.0	1.20	0.50	0.0	0.40	3.20
	SSS	0.40	0.40	1.40	5.80	2.80	0.90	0.90	1.30	0.0	0.50	0.20	3.40
	SCI	1.30	1.30	1.70	4.90	2.70	1.50	1.10	0.0	1.30	1.20	1.20	2.40
	COC	06.0	0.80	2.00	5.40	2.90	1.50	0.0	1.10	0.00	06.0	0.70	3.10
	<u> </u>	0.80	0.70	1.20	5.70	2.70	0.0	1.50	1.50	06.0	0.80	0.80	3.40
	INI	2.60	2.70	3.00	6.30	0.0	2.70	2.90	2.70	2.80	2.70	2.70	4.20
	GE	5.70	5.80	5.30	0.0	6.30	5.70	5.40	4.90	5.80	5.60	5.80	4.20
													3.50
	CAL	0.30	0.0	1.60	5.80	2.70	0.70	0.80	1.30	0.40	0.40	0.20	3.40
	AER	0.0	0.30	1.40	5.70	2.60	0.80	0.90	1.30	0.40	0.40	0.30	3.40
													DAT
						Independence	Avenue.	Site 11					

DAT 2.80	3.00	3.90	2.70	2.90	3.30	2.70	2.80	2.70	2.40	2.60	2.80	3.00	0.0
WAL 0.50	0.10	5.10	0.80	1.30	4.30	0.70	0.70	0.70	06.0	0.50	0.40	0.0	3.00
TSC 0.30	0.40	4.80	0.40	1.00	4.10	0.40	0.80	1.00	06.0	0.40	0.0	0.40	2.80
SSS 0.40	0.60	4.60	08.0	1.50	4.00	0.70	06.0	0.70	0.80	0.0	0.40	0.50	2.60
SCI	0.90	4.60	1.00	1.30	4.00	0.00	06.0	06.0	0.0	0.80	06.0	06.0	2.40
TOC	0.70	4.80	1.40	1.90	4.20	1.30	1.30	0.0	0.90	0.70	1.00	0.70	2.70
KAM 0 90	0.70	5.00	1.00	1.40	4.70	0.80	0.0	1.30	06.0	0.90	0.80	0.70	2.80
INT	0.70	4.70	0.40	0.70	4.10	0.0	0.80	1.30	0.90	0.70	0.40	0.70	2.70
GE A DO	4.40	2.80	4.00	4.00	0.0	4.10	4.70	4.20	4.00	4.00	4.10	4.30	3.30
ESL,	1.20	4.50	0.60	0.0	4.00	0.70	1.40	1.90	1.30	1.30	1.00	1.30	2.90
ERT 0 60	0.80	4.60	0.0	09.0	4.00	0.40	1.00	1.40	1.00	0.80	0.40	0.80	2.70
CEM	5.20	0.0	4.60	4.50	2.80	4.70	5.00	4.80	4.60	4.60	4.80	5.10	3.90
CAL	0.0	5.20	0.80	1.20	4.40	0.70	0.70	0.70	0.90	0.60	0.40	0.10	3.00
AER	0.40	4.80	0.60	1.10	4.00	0.60	0.90	0.90	1.00	0.40	0.30	0.50	2.80
A C C	CAL	CEM	ERT	ESL	GE	INT	KVM	1.00	SCI	SSS	TSC	WAL	DAT
				Military Road.	Site 14								

MATRIX OF CORRELATION COEFFICIENT OF MODEL PREDICTIONS TABLE 6-3

. Correlation Coefficient

MODELS

DAT	0.23	0 17	0 17	0.09	-0.04	0.20	0.27	0 22	0.22	0.27	0.24	0.0	
WAL	0.81	0.91	0.69	0.33	0.15	0.68	0.57	0.79	0.64	0.71	0.0	0.24	
TSC	0.78	0.67	0.87	0.31	0.22	0.60	0.41	0.43	0.69	0.0	0.71	0.27	
SSS	0.76	0.57	0.57	0.05	0.15	0.39	0.22	0.47	0.0	0.69	0.64	0.22	
SCI	0.54	0.72	0.39	0.25	0.08	0.50	0.50	0.0	0.47	0.43	0.79	0.22	
TOC	0.31	0.42	0.22	0.58	-0.07	0.18	0.0	0.50	0.22	0.41	0.57	0.27	
KAM	0.65	0.73	0.78	0.28	0.28	0.0	0.18	0.50	0.39	0.60	0.68	0.20	
INT	0.22	0.17	0.25	0.10	0.0	0.28	-0.07	0.08	0.15	0.22	0.15	-0.04	
GE	0.32	0.27	0.24	0.0	0.10	0.28	0.38	0.25	0.05	0.31	0.33	60.0	
ESL	0.75	0.72	0.0	0.24	0.25	0.78	0.22	0.39	0.57	0.87	0.69	0.17	
CAL	0.77	0.0	0.72	0.27	0.17	0.73	0.42	0.72	0.57	0.67	0.91	0.17	
AER	0.0	0.77	0.75	0.32	0.22	0.65	0.31	0.54	0.76	0.78	0.81	0.23	
	AER	CAL	EST	SE	INT	KAM	LOC	SCI	SSS	TSC	WAL	DAT	
					Independence	Avenue,	Site 11						

														2 0.25
TSC														
SSS	0.78	0.73	0.43	0.74	0.64	0.20	0.72	0.48	0.11	0.32	0.0	0.76	0.63	0.41
SCI	0.30	0.34	0.48	0.27	0.22	0.23	0.39	0.68	0.25	0.0	0.32	0.29	0.29	0.38
LOC	0.17	0.21	0.61	-0.10	-0.18	0.40	-0.07	-0.13	0.0	0.25	0.11	0.03	0.12	0.28
KAM	0.50	0.58	0.41	0.65	0.65	0.24	0.75	0.0	-0.13	0.68	0.48	0.62	0.57	0.32
INT	70.0	0.91	0.45	0.97	0.95	0.33	0.0	0.75	-0.07	0.39	0.72	0.97	0.88	0.33
GE	0.40	0.45	0.59	0.32	0.30	0.0	0.33	0.24	0.40	0.23	0.20	0.36	0.43	0.12
ESL	// 0	0.90	0.36	0.98	0.0	0.30	0.95	0.65	-0.18	0.22	0.64	96.0	0.88	0.24
ERT	0.00	0.93	0.41	0.0	0.98	0.32	0.97	0.65	-0.10	0.27	0.74	0.98	0.90	0.30
CEM	40.0	0.54	0.0	0.41	0.36	0.59	0.45	0.41	0.61	0.48	0.43	0.47	0.49	0.40
CAL	20.0	0.0	0.54	0.93	0.90	0.42	0.91	0.58	0.21	0.34	0.73	96.0	0.93	0.35
AER 0 0		0.83	0.54	0.83	0.77	0.40	0.82	0.50	0.17	0.30	0.78	0.85	0.72	0.38
AFR		CAL	CEM	ERT	EST	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL	DAT
						•	Military Road,	Site 14						

DAT 0.38 0.35 0.40 0.24 0.32 0.32 0.38 0.38 0.38 0.38 0.38

TABLE 6-4 CLUSTERING BY MEAN ABSOLUTE
DIFFERENCE BETWEEN MODEL PREDICTIONS

Mean Absolute Difference (ppm)	Site	Clusters
<0.2	11	(1) AER-WAL (2) CAL-WAL
	14	(1) CAL-WAL
<0.4	11	(1) AER-CAL-SSS-TSC-WAL
2	14	(1) AER-CAL-TSC-WAL (2) AER-ERT-TSC (3) ERT-ESL (4) ERT-INT-TSC
<0.6	11	(1) AER-CAL-SSS-TSC-WAL (2) AER-CAL-LOC-WAL (3) CAL-KAM
and the second s	14	(1) AER-CAL-ERT-INT-SSS-TSC-WAL (2) AER-CAL-LOC-WAL (3) CAL-LOC-WAL (4) ERT-ESL-INT-TSC
<0.8	11	(1) AER-CAL-KAM-SSS-TSC-WAL (2) AER-CAL-LOC-SSS-TSC-WAL (3) ESL-KAM-TSC
	14	(1) AER-CAL-ERT-ESL-INT-TSC-WAL (2) AER-CAL-ERT-INT-KAM-SSS-TSC-WAL (3) AER-CAL-INT-KAM-SCI-SSS-TSC-WAL (4) AER-CAL-KAM-LOC-SCI-SSS-TSC-WAL

TABLE 6-5 CLUSTERING BY 80TH PERCENTILE DIFFERENCE BETWEEN MODEL PREDICTIONS

80th Percentile Difference (ppm)	Site	Clusters
тете (рум)	Bite	Clusters
<0.2	11	(1) CAL-WAL (2) SSS-WAL
	14	(1) CAL-WAL
<0.4	11	(1) AER-CAL-TSC-WAL (2) AER-CAL-SSS-WAL
	14	(1) AER-CAL-TSC (2) AER-SSS-TSC (3) CAL-TSC-WAL (4) ERT-INT-TSC
<0.6	11	(1) AER-CAL-SSS-TSC-WAL
	14	(1) AER-CAL-SSS-TSC-WAL (2) AER-ERT-INT-TSC (3) ERT-ESL
<u><0.8</u>	11	(1) AER-CAL-KAM-TSC-WAL (2) AER-CAL-SSS-TSC-WAL (3) CAL-LOC-WAL
	14	(1) AER-CAL-ERT-INT-SSS-TSC-WAL (2) CAL-INT-KAM-TSC-WAL (3) CAL-LOC-SSS-WAL (4) ERT-ESL-INT (5) SCI-SSS

TABLE 6-6 CLUSTERING BY CORRELATION BETWEEN MODEL PREDICTIONS

Correlation Coefficient	Site	Clusters
>0.75	11	(1) AER-CAL-WAL (2) AER-ESL-TSC (3) AER-SSS (4) ESL-KAM (5) SCI-WAL
_	14	(1) AER-CAL-ERT-ESL-INT-TSC (2) AER-SSS-TSC (3) CAL-ERT-ESL-INT-TSC-WAL (4) INT-KAM
>0.65	11	(1) AER-CAL-ESL-TSC-WAL (2) AER-CAL-ESL-KAM-WAL (3) AER-SSS-TSC (4) CAL-SCI-WAL
-	14	(1) AER-CAL-ERT-ESL-INT-TSC-WAL (2) AER-CAL-ERT-INT-SSS-TSC (3) ERT-ESL-INT-KAM (4) KAM-SCI

total number of different models that cluster with each model is shown in the following tables: Mean Absolute Difference, Table 6-7; 80th Percentile Difference, Table 6-8; Correlation Coefficient, Table 6-9. Finally, Table 6-10 shows the grand total over all criteria from the previous three tables, for each model and distance measure.

Looking at Table 6-10, it is apparent that following four models cluster consistently under all the circumstances considered. AeroVironment (AER), California Division of Highways (CAL), TSC/EPA (TSC) and Walden Research (WAL). The Environmental Research and Technology (ERT) Model clustered well at the only site where it was run. The remaining models all failed to cluster as well as the above five. In particular, neither the General Electric (GE) nor the Center for the Environment and Man (CEM) models ever clustered with any of the other models. Again it should be emphasized that these results say nothing about the accuracy of the models.

Rased upon the above analysis five models appear to be members of the Consensus Cluster: AER, CAL, ERT, TSC, and WAL. It is interesting to note that three of these models are Gaussian (CAL, TSC, WAL) and two are Conservation of Mass (AER, ERT).

A wide variety of computer hardware was used in the running of the models studied here. For example, all in-house runs were made on an IBM 370/155; one contractor used a minicomputer; most contracters used largescale computers such as the Univac 1108, the IBM 360, 370 series, or a CDC model.

The amount of cpu(central processor unit)time used by companies participating in this study varied from a low of 7 seconds to a high of 2800 seconds. Computer use data are available for eight of the models tested in this study. These data are listed in Table 6-11.

In view of the different hourly rates charged for cpu time and the varying hardware and software used, it would not be fair to compare the cpu costs of the models run under contract. However, all five models tested in-house were run on the IBM 370/155, hence there is a comparability basis for these models. Assuming a \$700 per hour rate(including cpu time, disk I/O, core

TABLE 6-7 NUMBER OF MODELS CLUSTERING BY MEAN ABSOLUTE DIFFERENCE BETWEEN MODEL PREDICTIONS

Number of Different Models Clustering with Each Model

				Clust	ering	With	1 Ea	ich I	node.	L				
Mean Absolute Difference						MODI	ELS							
(ppm)	Site	ΛER	CAL	CEM	ERT	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL
<0.2	11	1	1	-	_	0	0	0	0	0	0	0	0	2
gastine .	14	0	1	0	0	0	0	0	0	0	0	0	0	1
<0.4	11	4	4	-	-	0	0	0	0	0	0	4 -	4	4
_	14	4	3	0	4	1	0	2	0	0	0	0	5	3
<0.6	11	5	6			0	0	0	1	3	0	4	4	5
_	14	7	8	0	7	3	0	8	5	2	0	6	8	8
<0.8	11	6	6	-	-	2	0	0	6	5	0	6	7	6
_ `	14	10	10	0	8	6	0	9	9	7	8	9	10	10
Total, Site	11	16	17	_	_	2	0	0	7	8	0	14	15	17
Total, Site	14	21	22	0	19	10	0	19	14	9	8	15	23	22
Grand Total		37	39	0	19	12	0	19	21	17	8	29	38	39

TABLE 6-8 NUMBER OF MODELS CLUSTERING BY 80th PERCENTILE DIFFERENCE BETWEEN MODEL PREDICTIONS

Number of Different Models Clustering with Each Model

TABLE 6-9 NUMBER OF MODELS CLUSTERING BY CORRELATION BETWEEN MODEL PREDICTIONS

Number of Different Models Clustering with Each Model

						MOI	DELS	3						
Correlation Coefficient	Site	AER	CAL	CEM	ERT	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL
>0.75	11	5	2	-	-	3	.0	0	1	0	1	1	2	3
20.73	14	6	6	0	6	6	0	7	1	0	0	2	7	5
>0.65	11	6	6	-	-	5	0	0	4	0	2	2	5	6
	14	7	7	0	8	7	0	8	4	0	1	5	7	6
Total, Site	11	11	8		-	8	0	0	5	0	3	3	7	9
Total, Site 14		13	13	0	14	13	0	15	5	0	1	7	14	11
Grand Total		24	21	0	14	21	0	15	10	0	4	10	21	20

TABLE 6-10 NUMBER OF MODELS CLUSTERING BY ALL DISTANCE MEASURES

Total Number of Different Models Clustering with Each Model

MODELS

	TOTAL		AER	CAL	СЕМ	ERT	ESL	GÉ	INT	KAM	LOC	SCI	SSS	TSC	WAL
	Site 11	20	40	40	-		10							34	
53 29 3 64 29 3	Site 14		49	51	0	46	26	0	47	23	12	10	35	56	48
	TOTALS		89	91	0	46	36	0	47	39	22	13	64	90	90

TABLE 6-11 COMPUTER USE

Company	CPU Time	(Secs.)	Computer Used
System, Science, Software	68		UNIVAC 1108
Lockheed Missiles and Space Company, Inc.	2800		UNIVAC 1108
Kaman Sciences Corporation	7	a 50 a	CDC CYBERNET 70
Environmental Systems Laboratory	70		IBM 370/155
General Electric	10		IBM 370/155
TSC/EPA	2300		IBM 370/155
California Division of Highways	60		IBM 370/155
Walden Research, Inc.	2000		IBM 370/155

memory,etc.),one could approximate the cost of running each of the in-house models with the synthetic data set used here. On this basis the TSC/EPA cost approximately \$470 to run,whereas the GE model cost only \$2.

It may be of some interest to relate the remaining models to the five members of the Consensus Cluster. To do this we computed the mean absolute difference between the "consensus" (the average of the predictions of the five Consensus Models) and the predictions of the remaining models. In addition, 10 percentage predictions exceeding the consensus of predictions was also calculated for each of the other models. These results are shown in Table 6-12. If the predictions of a model tend to exceed the average of the predictions of the Consensus Models, then model may be said to produce conservative estimates pollution. By this definition, INT, LOC, SCI, SSS, CEM and GE all produce conservative predictions. (However, predictions of CEM and GE are extremely the conservative since they almost always exceed the consensus predictions.)

should be noted that all of the above conclusions are based upon the results of running models with the reduced Airedale data set. Most of elements in this data set span a limited range values (as shown in Table 6-13) for only two configurations (both at-grade). Therefore, the Consensus Models identified above are, strictly speaking, only Consensus Models for input data in the ranges shown in Table 6-13 and for at-grade sites similar to the ones here. It is not clear that these same models will prove to be Consensus Models, defined at the beginning of this section, for other situations (such as receptors further from the highway, elevated 10 sections, different traffic or cut meteorological conditions, etc.).

Moreover, even within the range of the input data, the use of measured concentrations from part of the reduced Airedale data set for calibration purposes may have affected the overall clustering of those models which were calibrated to these data. (However, better calibration data will not exist for any set of synthetic data, or will they exist in many model applications, e.g., pollution estimations at sites not yet built.)

TABLE 6-12 DEVIATIONS OF OTHER MODEL PREDICTIONS FROM AVERAGE OF CONSENSUS MODEL PREDICTIONS

MODELS

	SITE	CEM	ESL	GE	INT	КАМ	LOC	SCI	SSS
Mean Absolute Difference (ppm)	11		0.89	3.93	1.68	0.61	0.58	0.98	0.32
	14	3.49	0.64	3.08	0.39	0.54	0.68	0.72	0.52
Percent Exceeding	11 14	99.2	39.0 47.1	99.8 100.0	54.5 62.1	47.6 43.3	68.3 66.7	97.0 82.1	54.2 83.8

TABLE 6-13 RANGE OF REDUC		E DATA ELEMENTS
DATA ELEMENT		MUMIXAM
WIND SPEED, mps	1	8
WIND ANGLE, deg.	0	360
STABILITY	2	7
TRAFFIC, vph	105	4303
VEHICLE SPEED, mph	34	39
RECEPTOR DISTANCE,	ft 36	48
RECEPTOR HEIGHT, ft	3	30

SITES: AT-GRADE

Thus, the findings of this report are only a first step toward identifying Consensus Models. Since no such information is presently available to Federal and state agencies, it was decided that the results of this preliminary study should be made available, even though they may be significantly altered by future tests. If, as seems likely, no suitable air quality data become available in the immediate future, clustering studies using synthetic data for a large range of variables and site configurations will be used to increase the range of applicability of the conclusions.

7. SUMMARY AND CONCLUSIONS

7-1 SUMMARY

- a. Thirteen highway air pollution dispersion models were tested, using the Airedale data base. Of these models, six were Gaussian, six were conservation of mass, and one was exponential.
- b. The Transportation Air Pollution Studies (TAPS) System was used in the testing process. The TAPS System is a package of computer programs for storing, manipulating, and retrieving air quality data, and for analyzing the performance of dispersion models by means of a series of statistical tests which determine the degree to which model predictions agree with measured air pollution.
- c. The initial purpose of these tests, which was to determine the accuracy of the models, had to be abandoned because it was found that the quality of the Airedale data is poor. Instead, it was decided to treat a portion of the Airedale data as a synthetic data set and to evaluate models in terms of how closely their predictions agree with one another.
- d. Three measures of the distance between model predictions were used; namely, the mean absolute difference, the 80th percentile difference, and the correlation coefficient. Models whose predictions fall within a defined cluster diameter are identified as Consensus Models.
- e. It is recognized that this is a preliminary analysis, based upon a data set with elements which span a limited range of values for only a single type of highway (at-grade). Hence, the conclusions stated below must be considered as tentative and subject to revision as further experiments with synthetic (or real) data are undertaken. However, since no such analysis is presently available to Federal and state agencies, it was felt that the results of this preliminary study should be made available at this time.

7.2 CONCLUSIONS

- a. Five models were tentatively identified as Consensus Models: AeroVironment (AER), California Division of Highways (CAL), Environmental Research and Technology (ERT), TSC/EPA (TSC), and Walden Research (WAL). Of these five models, three are Gaussian (CAL, TSC, WAL) and two are Conservation of Mass (AER, ERT).
- b. When compared to the five Consensus Models, six of the remaining eight models tended to overpredict pollution concentrations (i.e., tended to make conservative predictions).
- c. It is important to understand that the models identified here as Consensus Models are not necessarily more accurate than the other models. Accuracy can only be determined by evaluating the performance of the models on a suitable sample of highway air quality data. Such data do not exist at this time.
- d. The kind of evaluation reported here is useful to both Federal and state DOT officials who are concerned with the air quality impact of transportation. In particular, state highway engineers who select models from the group of Consensus Models for use in analyzing air quality may have a basis for defending their choice in any court case which might arise.
- e. These experiments have demonstrated that the Transportation Air Pollution Studies (TAPS) System is a gowerful tool for model testing. In particular, the TAPS System will allow the accuracy of models to be assessed on a production basis when suitable air quality data become available.

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February 12, 1974

APPENDIX A

TSC EXPLORATORY LETTER

Gentlemen:

TSC will soon be sponsoring a series of dispersion model validation experiments to be conducted in contractor plants using air pollution data supplied by the Center. This exploratory letter is being sent to you because of your expressed desire to participate in this exercise. Herein we specify the kind of input data to be furnished by TSC, the desired format of the output data which your company would supply us, the TSC model validation approach and the contractual arrangements under which the work will be funded.

The purpose of these experiments is to validate fully operational dispersion models, not to sponsor model R&D. Any work required to modify your model in order to accommodate the test data provided by TSC would be done at your own expense.

Input Data

The data to be supplied by TSC consist of traffic and meteorological parameters for two or more highway sites. The road types at these sites will consist of at least one at-grade highway and possibly a cut, or an elevated highway. Each site will be described in detail by TSC. Approximately five hundred cases will be supplied by TSC to each contractor. Some of these cases will include actual measured pollutant concentrations at receptors. These cases may be used for model calibration.

Each case will consist of hourly input data such as:

Site number

Meteorological parameters (e.g. wind speed, wind direction, stability, etc.)

Traffic parameters (e.g. vehicles per hour, vehicle speeds, etc.)

These data will be supplied on punch cards. For example, a typical set of cards for a case may contain the following data (with the site description and the receptor locations given separately):

Case number: 97

Site number: 3

Wind speed: 5mps

Wind direction: 272

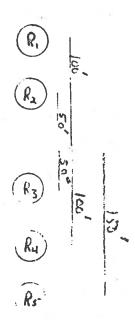
Stability:

Vehicles per hour: 472

Average vehicle speed: 47mph

Output Data

For each case, the desired output will consist of carbon monoxide concentration predictions at approximately 4 to 8 receptor locations. A typical receptor configuration might be the following:



The output data should be supplied on punch cards. The desired data format is:

CASE NUMBER	c_{i}	C_2	C,	 . C _M
rde 'e . e	• -	1	۰	. N
•	•		•	
•				

where $\mathbf{C}_{\mathbf{N}}$ is the concentration predicted at receptor N in parts per million for the case number shown.

Model Validation Approach

TSC has developed a sophisticated battery of statistical tests to measure the performance of dispersion models. One of these tests is based upon the decision theoretic approach which evaluates model performance in terms of its usefulness for decision-making. We will consider a simple go/no-go decision such that if \hat{C} >Cd decide high pollution and if \hat{C} <Cd decide low pollution, where \hat{C} is the model-computed

concentration and $C_{\rm d}$ is the decision-level concentration. If the losses associated with these two decisions are known it is possible to set up an integral defining the total loss which can be minimized by a proper choice of $C_{\rm d}$.

One of the ingredients of the loss integral is the conditional probability, $\Pr(C>C_1|\hat{C}=C_2)$, where C_1 and C_2 are arbitrary values of pollutant concentration, C is the measured concentration and \hat{C} is the corresponding concentration calculated by the model. (For example, C_1 might be the national primary ambient air quality standard for the pollutant in question.) This conditional probability is a "sufficient statistic" for selecting a model to be used in decision-making (it is, of course, not a single number but must be determined for all C_1 , C_2). TSC has developed a powerful statistical technique for estimating such probability.

In addition to the decision theoretic approach we will use some of the more conventional measures of performance. For example, we will construct several intuitive loss functions each of which stresses some aspect of the deviation between a pair of measured and computed concentrations. The summation of the loss function over data samples provides a single figure of merit for a model. Familiar examples of such loss functions are the mean square error and the mean log difference square error. We also intend to compute the rank correlation coefficient as a measure of the degree to which C and Ĉ increase together.

Thus each model will be subjected to a variety of tests which measure many aspects of its performance. Test results will be published in a series of reports which will be distributed to LOT, EPA and other interested agencies. These reports will be available to the public through NTIS.

Contractual Arrangements

TSC contemplates the issuance of unpriced purchase orders (with a "not to exceed" provision of \$2500) to those companies selected by the Government as a result of their affirmative response to this letter. Data will be forwarded to the contractors in mid-March. Delivery of contractor test results will be required within one (1) month following receipt of a purchase order. It is further noted that the Government will incorporate those clauses pertaining to either patents and/or data, as deemed appropriate.

Kindly use the attached form to indicate whether you wish to participate in these experiments and return same to the following address by February 22, 1974:

Department of Transportation Transportation Systems Center Kendall Square Cambridge, MA 02142 ATTN: Mr. Robert E. Valente, Code AWC

Should you desire any further technical information, please call Mr. Eugene M. Darling, Jr., (617) 494-2671.

Sincerely,

Robert E. Valente Contracting Officer

TRANSPORTATION SYSTEMS CENTER

Contractor Model Validation Experiments

	Company Name		
// will /		ate in the T	SC Contractor
Model Validation	Experiments.		
REMARKS:			
Signature			Date

March 22, 1974

APPENDIX B. TSC LETTER

TO EIGHT COMPANIES PARTICIPATING UNDER CONTRACT.
Gentlemen:

Thank you for your affirmative response in reply to our exploratory letter regarding your possible participation in the dispersion model validation experiments to be conducted by the Transportation Systems Center (TSC). A purchase order to cover computer expense related to running your dispersion model is being prepared by our Procurement Office and will be sent to you as soon as possible.

Enclosed you will find a deck of cards which is to comprise the air quality data to be used in this experiment. The format of these cards, as well as data definitions and their units, is explained elsewhere in this communication. Additionally, there is an accompanying sketch and description of each site at which data was gathered. Also to be found in this package are several model calibration or tune-up cases, if required by your model program.

It is requested that the output of your dispersion model be on punch cards with the concentrations in parts-per-million(ppm). A sample format card and an explanation are also enclosed. Please return the calibration test case results if used by your program.

Run as many cases as possible starting with site 11, being careful not to exceed the agreed upon maximum cost of \$2500. If you have further questions, please contact Eugene M. Darling at DOT/TSC.

6 Enclosures

INPUT DATA

COL.	FORTRAN FORMAT	DATA DEFINITION
4-5	12	SITE NUMBER
8-10	13	CASE NUMBER
17-20	14	VEHICLES PER HOUR
24-25	12	AVERAGE SPEED (mph)
30	I1	*STABILITY CLASS (1-7)
33-35	13	**WIND DIRECTION (deg.)
39-40	12	WIND SPEED (mps)
41-45	F5.1	UPWIND RECEPTOR 1 (ppm)
46-50	F5.1	UPWIND RECEPTOR 2 (ppm)
51-55	F5.1	UPWIND RECEPTOR 3 (ppm)

FORMAT (3X, I2, 2X, I3, 6X, I4, 3X, I2, 4X, I1, 2X, I3, 3X, I2, 3F5.1)

^{*1,2,3 -} UNSTABLE

^{4 -} NEUTRAL

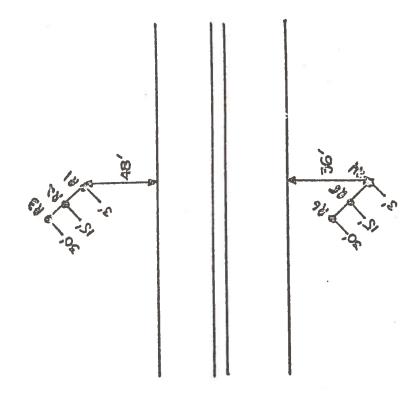
^{5,6,7 -} STABLE

^{**}WIND ANGLE IS MEASURED IN A CLOCKWISE DIRECTION WITH O° PERPENDICULAR TO THE ROAD.

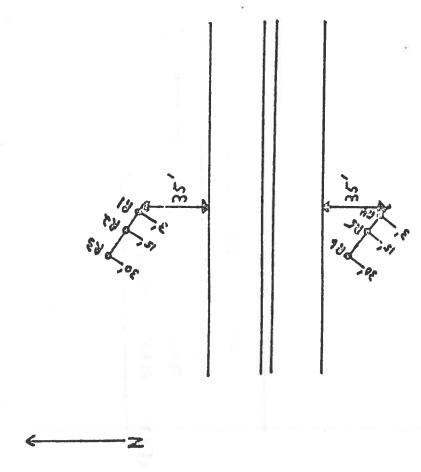
OUTPUT FORMAT

COL.	FORTRAN FORMAT	DATA DEFINITION
4-5	12	SITE NUMBER
8-10	13	CASE NUMBER
21-25	F5.1	DOWNWIND RECEPTOR 1 (ppm)
31-35	F5.1	DOWNWIND RECEPTOR 2 (ppm)
41-45	F5.1	DOWNWIND RECEPTOR 3 (ppm)
51-55	F5.1	DOWNWIND RECEPTOR 4 (ppm)
61-65	F5.1	DOWNWIND RECEPTOR 5 (ppm)

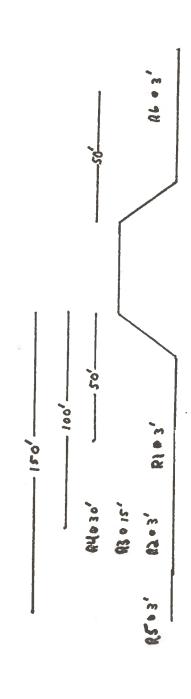
FORMAT (3X, 12, 2X, 13, 10X, 5(F5.1, 5X))



ב



SITE 14



SITE INFORMATION

SITE 11

Number of Lanes:

6

Highway Width:

72' (6-12' lanes)

Center Strip Width:

951

For wind angles between 0°-90° and between $270^{\circ}-360^{\circ}$, receptors R1, R2, R3 represent the background concentrations. For wind angles between $91^{\circ}-270^{\circ}$, receptors R4, R5, R6 represent the background concentrations.

SITE 14

Number of Lanes:

4

Highway Width:

52' (4-13' lanes)

Center Strip Width:

61

For wind angles between $0^{\circ}-90^{\circ}$ and between $270^{\circ}-360^{\circ}$, receptors R1, R2, R3 represent the background concentrations. For wind angles between $91^{\circ}-270^{\circ}$, receptors R4, R5, R6 represent the background concentration.

SITE 15

Number of Lanes:

4

Highway Width

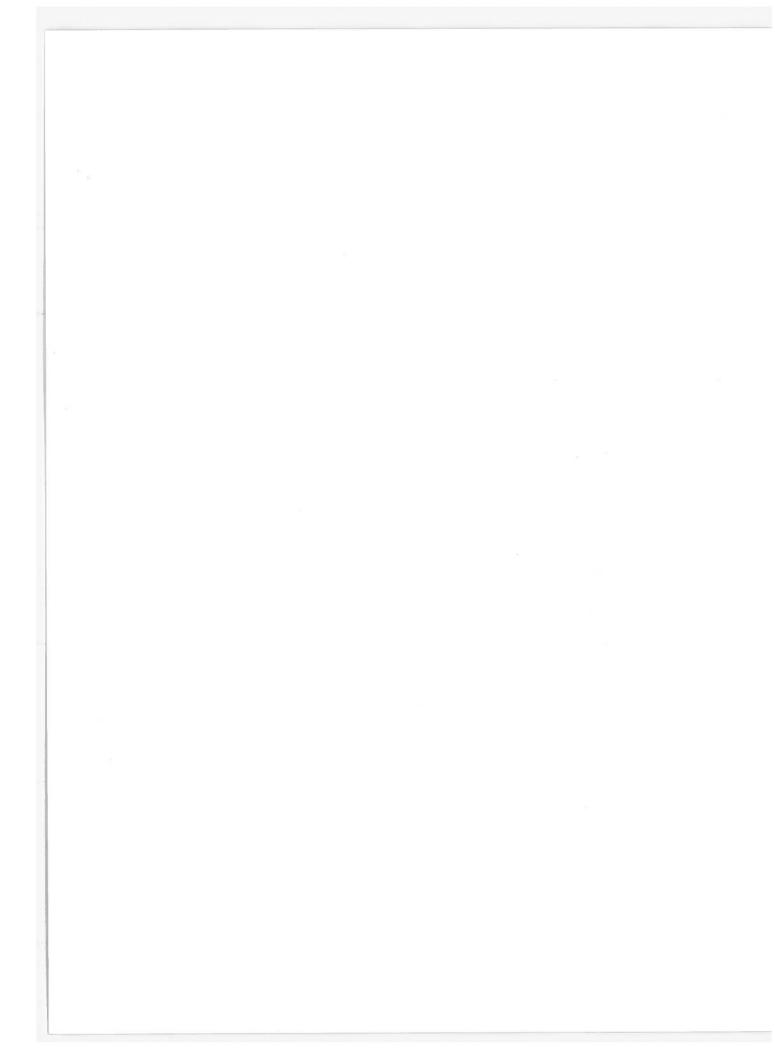
48' (4-12' lanes)

Center Strip Width:

13'

Height of Road Above Ground 25'

Receptors R1, R2, R3, R4 and R5 are always placed on the downwind side of the highway. Receptor R6 is always the background concentration and is positioned on the upwind side of the highway.



APPENDIX C. MODEL DESCRIPTIONS C.1 AEROVIRONMENT, INC. (AER)

The AeroVironment turbulent diffusion model was developed for air quality estimates for point or line source releases. The analytical details of the model are described in Ref. 1. This model is capable of handling any arrangement of sources for both steady and unsteady flows.

The basic turbulent diffusion mechanism is based on the short time asymptotic result of Taylor's diffusion theorem, thus the results are valid for distances less than about 3 km from the source. The spread of the plume, σ , varies linearly under an equation of the form $\sigma \sim$ at where a is the rms turbulence in an appropriate direction, and t the time of flight.

The rms turbulent velocities, a , are dependent on the surface roughness, the mean wind speed and conditions of atmospheric stratification expressed in terms of surface heat flux or stability parameters such as the Pasquill classes. A fundamental relation of turbulence generation is used to define a , given roughness, heat flux, and wind speed.

The unsteady partial differential equation for concentration is formulated with transfer coefficients expressed from Taylor's result. A fundamental solution is obtained which can be exactly integrated both in time and space. For a steady line source the basic result is that concentration varies approximately inversely with wind speed and downstream distance, while the vertical distribution is very close to Gaussian.

Ref. 1. Lissaman, P. B. S., A Simple, Unsteady Concentration Model, Explicitly Incorporating Ground Roughness and Heat Flux. Preprint No. 73-129, Air Pollution Control Association Meeting, Chicago, June 1973.

This model has been given the name AVQUAL. Because of its speed and simplicity, the model can be readily operated on minicomputers and a number of different programs have been developed for the Hewlett-Packard 9820A computer. To generate data cards compatible with the DOT validation exercise, AVQUAL has also been programmed in FORTRAN to run on an IBM 360/50.

¢.2 CALIFORNIA DIVISION OF HIGHWAYS (CAL)

INTRODUCTION

This computer program calculates the pollutant concentrations generated by motor vehicles within a highway corridor. The mathematical model, which is based on the Gaussian Diffusion Equation, calculates hourly concentrations of pollutants within the mechanical mixing cell as well at receptor points at given distances from the roadway. The computerized model is capable of estimating pollutant concentrations where the winds are either parallel or at an angle to the highway alignment and where the highway section may be at grade, elevated or in a cut.

This User's Guide is intended primarily to assist users in preparing input data for the computer program. It does not constitute a complete documentation of the program nor an instruction manual for its application. Prospective users should be thoroughly familiar with the contents of a report titled "Mathematical Approach to Estimating Highway Impact on Air Quality" (heport Number FHWA-RD-72-36) and an accompanying Appendix (FHWA-RD-72-37) before attempting to use the program. Report Number 72-36 describes the mathematical formulation, basic assumptions and limitations of the model that is the basis of the computer program. Report 72-36 also contains several problems that have been computed manually illustrating how the model may be applied.

CORRIDOR ANALYSIS

Mathematical Assumptions

The mathematical model presented in this manual is based primarily on the Gaussian Diffusion Equation, that is, the concentrations of pollutants within the plume generated by the vehicles on highways are distributed normally in both the cross-wind and vertical directions. The following are other basic assumptions that went into the development of the mathematical model for highway line sources:

- Continuous emission sources from vehicles on highways for the time period analyzed.
- 2. The surface stability classes of the atmosphere are determined from studies made by Pasquill [1] and from an objective system of classifying stabilities from meteorological observations as suggested by Turner [2].
- 3. The concentration of pollutants on highways within the mechanical mixing cell is independent of surface stability classes. The mechanical mixing cell can be defined as the area on the misney where there is in intense tone of mixing and turbulence caused by the movies of the vehicles. The vertical height of the mixing cell is assumed to be 12 feet. The horizontal width of the mechanical mixing cell is assumed to extend from edge of shoulder to edge of shoulder for medians less than or equal to 30 feet.
- A uniform wind flow field exists, that is, there is no variation of wind speed with height (wind shear).
- No aerodynamic effects on air passing over structures, buildings, and other obstructions.

Further discussion of these assumptions along with the limitations and applications is presented later. .

Calculations for Crosswinds

Mixing Cell Concentrations

The concentration of pollutants on the highway within the mechanical mixing cell for highways located on elevated, cut, or at-grade sections may be estimated (for any surface stability class) by using the following equation for Ø greater than 12°:

$$C = \frac{1.06 \, Q}{K_1 \, \overline{u} \, \sin \, Q}$$
 (3)

Where $C = Concentration of pollutant <math>gm/m^3$

Q = Emission source gm/sec-m

 \overline{U} = Wind speed m/sec (1 mph = 0.447 m/sec)*

K₁ = Empirical coefficient determined by field measurements**.

Ø = Angle of wind with respect to highway alignment as
 determined from the computer program [5] WNDROS or
 STAROS based on a 16 point compass reporting system.
Ø will be one of the following angles using the
 highway alignment as a reference or base line:

 $g = 22.5^{\circ}$

Ø = 45°

 $\emptyset = 67.5^{\circ}$

 $\emptyset = 50^{\circ}$ (wind direction is perpendicular to highway alignment).

1.06 = Empirical factor relating the height of the mechanical mixing cell to concentration

To compute the source strength term Q in equation 3 use the following equation:

 $Q = [1.73 \times 10^{-7}] \times [vehicles per hour] \times [emission factor] (4)$

Where the numerical constant is a factor to convert the units of the product (vph)(gm/mi) to gm/m-sec.

*The minimum recommended wind speed is 2 mph or about 1 m/sec.

**Until sufficient data become available from the Division of Highways Research Project [10] assume $K_1 = 4.24$.

The emission factor used in equation 4 depends on the model year, emission standards, percentage of HDV, average route speed, etc.

Values are given by Beaton et al [4] for the primary pollutants emitted by the motor vehicles.

The calculated concentration from equation 3 should be converted to parts per million concentrations by using equation (1).

INPUT

This section describes the formats and input data required by the computer program.

The required inputs to the mathematical model to estimate hourly pollution concentrations on and within the highway corridor are described below:

- 1) Traffic volume in number of vehicles per hour.
- Emission factors of vehicles using the highway as a function of heavy duty vehicle (HDV) mix and average route speed.

- 3) Meteorological parameters, that is, surface stability of the atmosphere and its associated probability of occurrence along with its corresponding wind rose.
- 4) Type of highway design, that is, a highway located on a fill or viaduct section, cut section, at grade section, etc.
- Horizontal and vertical dispersion parameters.

Each of the above inputs into the mathematical model is discussed in detail below.

Traffic

The traffic input data for a proposed highway normally will be the peak and off-peak hourly volumes and their associated time of occurrence. This information can be obtained from District Traffic or Urban Planning Departments and will cover the period from the estimated time of completion of the proposed highway to twenty years thereafter. This is discussed in detail in a report by this department [3].

Emission Factors

The input emission factors [4] for carbon monoxide for the estimated time of completion and ewency years nence can be obtained from reference [4] depending on the percentage of Heavy Duty Vehicles (HDV) and the average route speed. If the estimated HDV mix does not correspond to the exact value used in the figures of reference [4] use a direct linear interpolation between the lower and higher HDV mix to obtain a value for the emission factor.

Wind Speed, Direction, and Stability

The output from the computer program [5] WNDROS or STAROS* will give for a specified time, (1) the probability of occurrence for each surface stability Class A through F inclusively and (2) the wind roses for the associated surface stability classes. Stability Class A is the most favorable meteorological condition in terms of the dispersion of pollutants while Stability Class F is the most unfavorable (worst) meteorological condition and results in the highest ground level concentrations. For a quantitative air quality study, it is necessary to compare two meteorological conditions which are obtained from the computer programs WNDROS or STAROS*. The two conditions are (1) the most probable

^{*}The STAR2 computer program has replaced the STAROS program.

surface stability class and its associated wind rose, and (2) the most unfavorable, or worst meteorological conditions its probability of occurrence, and its associated wind rose. The most probable and the worst meteorological conditions are usually estimated for the time periods when the peak and off-peak traffic hours occur. This is discussed in detail in a report by Beaton et al [5].

Type of Highway Design

The input for the type of highway design consists of one of the following:

- 1. at grade section
- elevated highways 30 feet or less
- 3. elevated highways over 30 feet
- 4. cut section

For each of the above types of design, with the exception of the at grade section, the height of fill, viaduct, or elevated section must be determined. The same applies to the cut section, that is, the depth of cut must be determined. The geometric characteristics can be obtained from plans furnished by the Design Section.

Horizontal and Vertical Dispersion Parameters

The horizontal and vertical dispersion parameters are used in the mathematical model to characterize the transport and dispersion of pollutants for different meteorological conditions.

These dispersion parameters are a measure of the surface stability of the atmosphere which greatly influences the ground level concentrations. Figures 86 and 87 in Appendix* are plots of the vertical and horizontal dispersion parameters. The use of these parameters is illustrated in Example 2.

The following describes the input data layout required by the program:

Card Number 1 (Always Required)

Punch an X in card column 1 to select the cross wind calculations. Punch a P in card column 2 for parallel wind calculations. Punch an X and a P in the respective columns for both calculations.

Card Number 2 (Cross wind input data) (All data right justified)

Card Columns	Format	Symbol		Description
1-10	F10.0	VPH		Vehicles per hour
11-15	F.5.0	EF		Emission Factor (Grams per mile)
16-20	F 5.0	υ		Wind speed (Miles per hour)
21-25	F 5.0	PHI		Wind angle (Degroos)
26-30	F 5.0	H		Pavement Height (Feet)
31 - 35	F 5.0	• 2	×	Receptor Height (Feet)
36-40	F 5.0	D	٠	Distance from edge of Shoulder to receptor (Feet)
41-42	I 2	CLAS		Stability Class (1-6 = A-F)
43-51	F 9.0	MW	/	Molecular Weight of Pollutant
52- 80°		(Leave Blank)		,2

Card Number 3 (Parallel wind input data) (All data right justified)

			10.000
Card · Columns	· Format	Symbol Symbol	Description
1-10	F10.0	VPH	Vehicles per hour
11-15	F 5.0	EF ·	Emission Factor (Gram per mile)
16-20	F 5.0	σ	Wind Speed (Miles per hour)
21-25	F 5.0	PHI	Wind angle (Degrees)
26-30	F 5.0	H	Pavement height (Feet)
31 –35	F 5.0	. Z	Receptor height (Feet)
36-40	F 5.0	D	Distance from edge of shoulder to receptor (Feet)
41-42	I 2	CLAS	Stability Class (1-6 = A-F)
43-51	F 9.0	W	Molecular Weight of Pollutant
52-60	F 9.0	DMD	Downwind distance from point
	*		where wind initially becomes parallel to highway (Feet)
61-69	F 9.0	W	Width of highway, shoulder to shoulder (Feet)
70-78	F 9.0	. WDTH	Average width of cut (Average of top and bottom widths in feet)
79-80		(Leave Hanle)	2

OUTPUT

The output of the mathematical model is a series of curves (Figures 1 to 85 in Appendix). These curves are a plot of the ground level concentration ratio CuK/Q versus the downwind distance. From these curves estimates of hourly concentrations of carbon monoxide can be made for the highway corridor region. These values are solely due to vehicle emissions and must be added to background concentrations to obtain total pollutant concentration levels.

*The appendix for this volume is published scharately

These appendix curves are divided into four basic groups as described below: .

- Group 1: Appendix Figures 1 to 6 are for at grade sections where the wind is not parallel to the highway alignment.
- Group 2: Appendix Figures 7 to 54 are for elevated sections, that is, fills, viaducts, and bridges where the wind is not parallel to the highway alignment.
- Group 3: Appendix Figures 55 to 78 are for cut sections where the wind is not parallel to the highway alignment. These curves can be used to estimate the concentrations of pollutants generated by highways with shallow cuts. (Depth of cut < 30 feet.)</p>
- Group 4: Appendix Figures 79 to 85 are for highway sections where the wind is parallel to the highway alignment.

The curves in Appendix Figures 7 to 54 indicate the theoretical relative difference in ground level concentrations for highways on elevated sections compared to at-grade sections. In these figures the curve for H=O represents the at-grade section for winds not parallel to the highway alignment. Detailed field measurements are required to validate this reduction in ground level concentration for elevated sections, however, the relative effects can be seen from the curves. The same reasoning applies to the comparison between at-grade sections and cut sections shown in Appendix Figures 1 to 6 and Appendix Figures 55 to 78, where the winds are not parallel to the highway alignment and for different surface stability classes.

In Appendix Figures 1 through 78 where the winds are not parallel to the highway, the angle of intersection (Ø) between wind direction and the highway centerline has the following application:

- Ø = 22.5° corresponds to angles from 12° to 33°
- \emptyset = 45° corresponds to angles from 34° to 56°
- \emptyset = 67.5° corresponds to angles from 57° to 78°
- $. \emptyset = 90^{\circ}$ corresponds to angles from 79° to 101°

Appendix Figures 79 through 85 (where the winds are parallel to the highway slignment) are used where the angle of intersection (Ø) between the wind direction and highway centerline is less than 12°.

Figure 1 illustrates the wind direction and ranges.

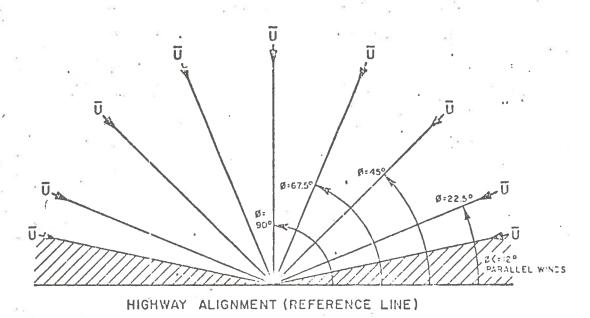


Fig. 1 ANGLE OF INTERSECTION BETWEEN WIND DIRECTION
AND HIGHWAY ALIGNMENT IN DEGREES

.The variables* on the curves in the Appendix are:

- C = Concentration of pollutant in grams per cubic meter (gm/m³)
- $\overline{\overline{\mathbf{U}}}' = \mathbf{Mean}$ surface wind speed (m/sec) **
- $Q = Emission source strength <math>\frac{cm}{sec}$ (winds parallel)
 and

gm sec-m (winds not parallel)

K = Empirical coefficient determined by field measurements

Until sufficient data become available from the Division of Highways research project [10] assume K = 4.24 on all curves.

The system of units for concentrations should be consistent with the California Air Quality Standards in parts per million by volume or the Environmental Protection Agency Standards in micrograms per cubic meter. The following equations convert the concentration from the curves in grams per cubic meter to parts per million by volume based on a reference temperature of 25°C and pressure of 760 mm of mercury, and from grams per cubic meter to micrograms per cubic meter.

$$ppm = \mu g/m^3 \frac{(0.0245)}{M.W.}$$
 (1)

Where ppm = Concentration of pollutant in parts per million by colume .

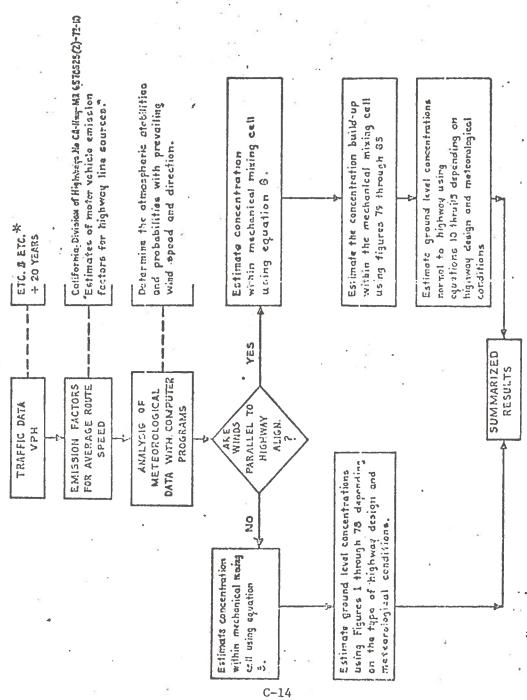
 $\mu gm/m^3 = Concentration of pollutant in micrograms per cubic meter$

$$1 \mu gm/m^3 = 10^{-6} gms/m^3$$
 (2)

M.W. = Molecular weight of the pollutant.

*All units used in the model equations are in the metric system.

**Ū is representative of the undisturbed air flow measured at a height of 10 meters above the ground surface over flat level terrain or modified for surface roughness as defined in reference [5].



*ETC= Estimated Time at completion."

Fig. 3. Systems flow chart for highway line course disnersion model

SUMMARY

The mathematical analysis of the impact of a highway on the environment requires two analyses: (1) corridor analysis and (2) mesoscale analysis. In the corridor analysis, special consideration is given to estimating the CO pollutant concentrations from the highway to the point downwind where ambient levels are again approached. The mesoscale analysis emphasizes the "air basin concept". This analysis evaluates the effects of the proposed highway on general community air quality. Consideration is limited, at the present, to two primary gaseous pollutants emitted from motor vehicles namely CO and HC.

At the present time the California Division of Highways has concentrated most of its efforts in developing and validating a mathematical model for the highway corridor region. More extensive work with actual field measurement of pollutant concentrations will be made in the future to develop and statistically validate regional models to supplement the present mesoscale analysis.

Figures 14 and 15 are generalized flow charts for the corridor and mesoscale analysis along with the required inputs.

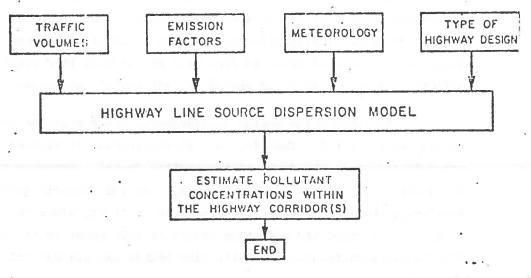


Fig. 14 FLOW CHART FOR CORRIDOR ANALYSIS

- C.3 CENTER FOR THE ENVIRONMENT AND MAN (CEM)
- TO: United States Department of Transportation Transportation Systems Center
- RE: The CEM Highway Traffic Air Pollution Model

The Analysis

Highway traffic air pollution sources and receptor locations are defined as a set of discrete x, y, z points. Each source point represents an area of unit pollutant emission. For the present case, emissions are assumed uniform in the relevant stretch of highway; thus, source points are uniformly spaced down the centerline of each traffic lane.

Pollutant diffusion in the direction of the wind is ignored. It would only be relevant if time variations in emission rate were known. Horizontal diffusion lateral to the wind is assumed to uniformly fill a \pm 10° azimuthal sector centered on the wind direction. This approximation to Gaussian diffusion is realistic and is made for convenience and efficiency. Since the model uses a multi-discrete-point source representation of a line source representation of the true traffic source configuration, the exact form of the lateral dispersion function is of little consequence. Vertical dispersion is assumed Gaussian from real and virtual (for ground-reflected pollution) sources displaced upwind to 'effective' locations.

To compute the upwind displacement, the turbulence depth at the roadway is estimated. That is, σ_z at the roadway is assumed to have a value dependent on the depth of the traffic 'wake'. Assuming this $\sigma_{z_0}(R_0)$ the displacement is the corresponding R_0 from the Pasquill curves. Similarly, the source height is assumed to be 10 ft, since the turbulence is assumed to raise the effective source to some point in the traffic wake. For the elevated roadbed, the effective height was assumed only 5 ft above the surface.

Since the highway was assumed uniform in both directions from the test site, source points were only defined in one direction from the test

(contd) The CEM Highway Traffic Air Pollution Model

site (except a short distance the other way to allow for plume spreading for winds nearly normal to the highway). The wind component normal to the highway then determined which receptors were downwind and the absolute value of the component along the highway was used to get the correct concentration from the one-sided set of sources. A \pm 10° sector upwind from each receptor determined the affective sources. Only contributions from those sources were computed.

A numerical fit to the Pasquill stability curves was made to give the constants of a three parameter empirical form. These constants were used in the program to generate a σ_Z (R, STABILITY) table from which σ_Z 's were extracted as needed. Five categories were used (Pasquill B-F) corresponding to the given 2-6. Given categories 1 and 2 were called 1, categories 3-6 were called 2-5 and 7 was also 5. Emission source strength was computed for highway traffic using the EPA average emission factor for Carbon Monoxide for 1973 based on nationwide statistics (62 G/vehicle-mile) multiplied by a speed correction factor $\frac{10.6}{(\text{SPEED}).8}$ which is a numerical fit to the EPA curve for average speed correction factors for all model years.

Execution

The program was written in ANAL70 (a CEM language) for execution on a UNIVAC 1108. The program consists of 45 lines of code, plus the data cards. Storage is automatically assigned by the language and does require access to a drum. Output consists of a printed tabulation of results. Tape and graphical display output can be generated with one or two more lines of code. The program can handle 1484 cases at a time without modification. Ten seconds were used to initialize the language, 16 seconds to compile the present program, 2 seconds for preliminary computations and approximately 1/2 sec per case for the final computations. One hundred and fifty-nine cases were run (all calibration cases, plus data runs for sites 14 and 15 only) for a total execution time of 1 min 42 sec.

(Cost = \$14.40)

The Program

The program consists of initial system array definitions followed by -

- Read data cards (DEP cards with 10 values each)
- Pre-process data
 - o convert site numbers 11, 14, 15 to 1, 2, 3
 - o convert wind directions 0 to 360° from y axis to 0 to \pm 90° from X axis in each quadrant
 - o set wind direction always + at site 3 (15).
 - o convert stability classes 1 through 7 to 1 through 5
 - o divide traffic count (VPH) by number of lanes to get VPH/lane
- Read y coordinates of traffic lanes, receptors
- Compute relative radius, azimuth between all source, receptor combinations
- Read z coordinates of each receptor, H of each site compute ($z \pm H$) for each receptor
- Read stability coefficients Compute sigma z as function of stability, radius
- Compute $\frac{Q}{\sqrt{2\pi} \left(\frac{\Delta\theta \cdot R}{360}\right)} \left\{ \exp \left[-\frac{1}{2} \left(\frac{Z-H}{\sigma_z} \right)^2 \right] + \exp \left[-\frac{1}{2} \left(\frac{Z+H}{\sigma_z} \right)^2 \right] \right\}$
- Compute for each case
 - o Extract relative radius, aziliuth tables and Gaussian function for this site
 - o Determine all source points for which wind direction minus relative azimuth of source, receptor is less than $10^\circ = \Delta\theta$
 - o Correct Q for VPH, SPEED for this case
 - o Divide plume function by $(\sigma_z \cdot WIND SPEED)$
 - o Add effective source displacement to table of relative radii
 - o Add to the background concentration the plume function at each receptor for correct relative radius from each source which is within ± 10° upwind sector.
 - o Store answers for this case
- Print table of pollutant concentrations for all cases for all receptors.

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       ) CENTER FOR THE ENVIRONMENT AND VAN, INC

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             ) TELEPHONE 203 549 4400 EXT.390
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C.4 ENVIRONMENTAL RESEARCH AND TECHNOLOGY (ERT)

DESCRIPTION OF THE EGAMA HIGHWAY AIR POLLUTION MODEL ENVIRONMENTAL RESEARCH AND TECHNOLOGY, INC.

429 Marrett Road

Lexington, Massachusetts 02173

1. INTRODUCTION

The Egan-Mahoney advection-diffusion Modeling program is applicable to a study of the dispersion of vehicular emissions in the near field of highways. The program numerically simulates the primary dispersion mechanisms of emissions from highway sources throughout a "two-dimensional" grid system and computes pollutant concentrations for each grid element.

The capability of treating spatially varying winds - both horizontal and vertical - and diffusivities is a major feature of the model. The wind fields and diffusion coefficients can be internally calculated as a function of highway geometry or, if otherwise available, can be read into the program. The geometry can be specified to represent at-grade, elevated, or depressed highway sections. The concentrations are predicted with a forward time step routine until a steady-state solution is reached.

This numerical dispersion model has been developed in the FORTRAN IV computing language and is called EGAMA in the ERT program library.

2. MODEL DESCRIPTION

2.1 The Tracer Equation

The advection and diffusion of a pollutant are governed by the tracer equation. The two-dimensional equation, used in this study, describing the change of concentrations resulting from horizontal advection, vertical advection, vertical diffusion, and source emission is:

$$\frac{\partial \chi}{\partial t} = U \frac{\partial \chi}{\partial x} - W \frac{\partial \chi}{\partial z} + \frac{\partial}{\partial z} (K \frac{\partial \chi}{\partial z}) + Q$$

where:

```
(x,z) are the downwind and vertical directions (meters) in a two-dimensional Cartesian system,

\chi is the concentration of the particular pollutant in g/m^3,

t is time (seconds),

U(x,z) is the horisontal wind (msec<sup>-1</sup>),

W(x,z) is the vertical velocity (msec<sup>-1</sup>),

K(x,z) is the turbulent diffusivity (m<sup>2</sup> sec<sup>-1</sup>),

and Q is the source emission rate (g/m^3/\text{sec}),
```

To simulate pollutant dispersion across and downwind of a highway, a vertical cross-sectional region enclosing the highway is divided into a number of grid elements; and the partial derivatives in the tracer equation are approximated by finite differences corresponding to the dimensions of the two-dimensional grid elements.

If the horizontal dimensions of the grid elements are set equal to the width of a road lane and the vertical dimensions equal to a mean initial mixing depth for the aerodynamic wake region of the vehicles, traffic in different lanes can then be represented by volume source emission rates in the corresponding grid elements. Boundary conditions and initial values of the concentration field need to be specified for the grid cell representation For most applications, the initial values of the concentration field are equal to zero. The steady-state solution is then generated from the rest. Howeve current pollution levels and upwind background levels can be used as initial values and boundary values for special situations.

2.2 Horizontal and Vertical Advection

The finite-difference simulation for horizontal advection, vertical advection and vertical mixing in the governing equation is performed in thre separate, sequential steps in the computation procedure.

Conventional finite-difference approximations to the two advection terms Uax/ax and Wax/az, produce truncation errors which, in effect, introduce numerical "pseudo-diffusion," errors into the predicted quantities. This artificial upwind and downwind mixing rate of the material by the numerical scheme can be orders of magnitude larger than that resulting from the real atmospheric mixing process.

The pseudo-diffusion associated with the numerical advection term can be substantially reduced by utilization of one or more statistical moments of the concentration distribution within a grid element in the computation scheme. A description of the use of statistical moments in finite difference calculations may be found in Egan and Mahoney (1972) (Reference 1).

2.3 Vertical Diffusion

The vertical diffusion component, $\partial/\partial z(K \partial \chi/\partial z)$, is simulated by a forward-time, centered-difference technique modified so that variable grid spacing can be specified in the vertical. In regions where parameters or concentrations change rapidly with height, resolution and accuracy can be improved with smaller vertical grid spacing. In other regions where gradients are smaller, large grid spacings can be used. Details of the computational routine which involve the conservation of the first and second moments of the horizontal distribution may also be found in Reference 1.

2.4 The Two-Dimensional Grid System

Figure la illustrates the basic forms of the wind and turbulent diffusivity fields expected for a depressed highway section. Figure 1b illustrates the two-dimensional grid field representation used for computation purposes in the model.

The grid system is defined on a two-dimensional Cartesian coordinate system with the abscissa as the horizontal axis and the ordinate as the vertical axis. The length of the system is the total number of horizontal grid elements multiplied by Δx , the horizontal dimension of a single grid. z_{n+1} determines the height of the top of the nth vertical element. The vertical dimension of the nth cell is \mathbf{z}_{n+1} - \mathbf{z}_n . As is seen on Figure 1b, the horizontal (U) velocities are calculated at the left and right sides of an element while the diffusivities (K) and vertical velocities (W) are defined at the top and bottom of an element. The basic flow is always assumed to be from left to right. The model allows for three boundary obstacles as simulations of the various highway configurations. These are shown in Figure 1 by the hatched areas. These three obstacles are independent and may be specified individually or together. The two outer obstacles with the four boundaries desired a kinematic boundary condition of U=0, W=0, and K=0. The inner obstacle (h_3, l_3) is transparent to the winds, but diffusivities downwind are altered by its presence.

5 Calculation of the Wind Field

Both the horizontal, U(x,z), and vertical W(x,z), winds are calculated on the basis of conservation of mass and according to the "topography" in the grid system. A simple power law expression for U is assumed to be valid at the left boundary, i.e., $U(x = 0, z) = U_1(z/z_1)^{\alpha}$, where

- U₁ is a measured wind speed,
- z_1 is the height at which U_1 is measured,

and

α is an externally imposed parameter depending on atmospheric stability conditions.

For computational purposes the wind direction is always perpendicular to the highway. To simulate the effect on concentrations of winds at small azimuth angles (θ) from the normal (θ = o with perpendicular winds), the model reduces the wind speed in the advection terms by a factor cos 0. This medification in essence simulates the effects of oblique wind angles on increasing the travel time of pollutants to corresponding positions normal to the roadway and on increasing the source emissions per unit time into the flow over the roadway. The procedure is valid for θ less than about 45°. The wind fields for different obstacle configurations are calculated by assuming that various horizontal velocity profile modifications will result from the presence of obstacle: to the flow and by requiring that the wind fields that result satisfy corservation of mass at each grid element. The fields calculated are expected to be valid for typical freeway cross sections where the roadway width is large with respect to the roadway depression depth. Certain constraints are imposed to limit the use of the computation schemes to the calculation of wind fields to sections of this type.

The model was extensively validated for near highway concentration estimates in a study performed for the District of Columbia Department of Highways and Traffic (References 2 and 3).

INPUT

- 1. Dimensions of grid system
- 2. Dimensions of grid elements
- 3. Cross wind angle
- 4. Wind speed
- 5. Stability
- 6. Dimensions of boundary obstacles
- 7. Source Emission Rates (g/m/sec)

OUTPUT

- 1. Horizontal wind field
- 2. Vertical wind field
- 3. Diffusion coefficients for each grid element
- 4. Emissions field (by grid element)
- 5. Concentration field (by grid element)

REFERENCES

- Egan, B. A. and J. R. Mahoney, 1972: Numerical Modeling of Advection and and Diffusion of Urban Area Source Pollutants, <u>J. Appl. Meteor.</u>, 11. 312-322.
- 'Development of Procedures to Simulate Motor Vehicle Pollution Levels', ERT Document P-343-F Environmental Research and Technology, Inc., Lexington, Mass. February 1973.
- Egan, B. A. and T. F. Lavery, 1973: Highway Designs and Air Pollution Potential. Presented at the AIAA Third Urban Technology Conference. Boston, Massachusetts, 26-28 September 1973.

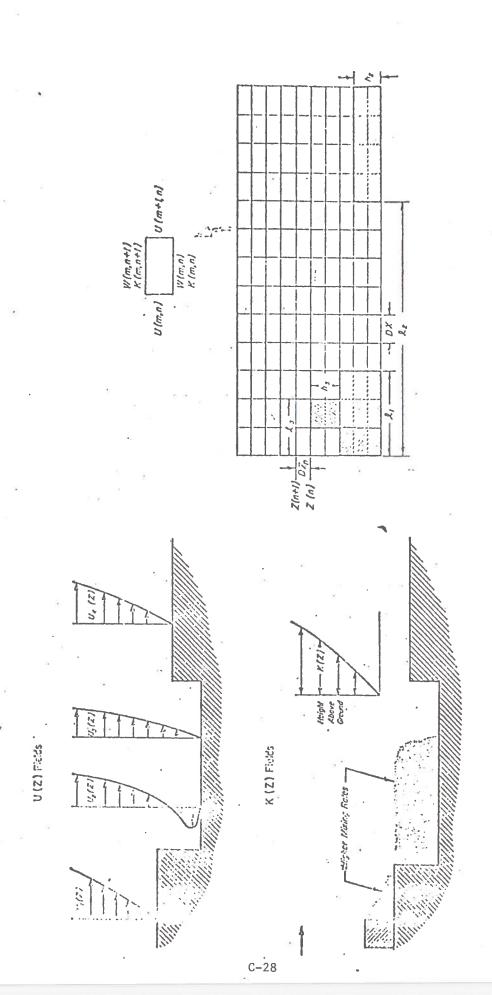


Figure 1-b The Two Dimensional Grid Field

Figure 1-a Wind and Diffusivity Fields

C.5 ENVIRONMENTAL SYSTEMS LABORATORY (ESL)

ESL HIGHWAY MICROSCALE DISPERSAL MODEL

The ESL Highway Microscale Dispersal Model has been designed to provide accurate and rapid calculations of air pollutant (non-reactive gases and particulates) concentrations from highway traffic. The model has been calibrated and validated using field measurements of carbon monoxide and particulates (especially lead). In the model, the fundamental Gaussian dispersal equation is employed to calculate atmospheric diffusion and transport. A formulation of this type provides for rapid computer calculations which require a minimum amount of computer storage capacity. Readily available tabulations of the error function and the normal cumulative distribution function are employed in the model. For convenience the model requires only the normally available traffic, geometric, and meteorological parameters:

- Traf::ic Data (vehicle classification mix, age mix, and speed)
- Roadway Geometry (cut, at-grade, elevated distance between roadway surface and ground)
- 3. Meteorological Conditions (calm or definite wind speed, wind direction, and Pasquill Turbulence Classification).

NOTE: In contrast to many Gaussian Models, the ESL model accepts calms and winds parallel to the roadway.

In addition to the above parameters, highway air pollution dispersal involves such processes as the mechanical generation of turbulence by high-speed vehicles and the absorption of vehicular emissions by the ground. The ESL model incorporates these effects as described below.

Model Description.

The ESL model uses the fundamental Gaussian plume model for a continuous elevated non-reactive point source to calculate the dispersal, transport, and precipitation of vehicular emissions in the atmosphere near the roadway. The general form of this equation, using the coordinate system described in Figure 1, is:

$$\overline{\chi}(x,y,z) = \frac{Q}{2\pi \overline{u}\sigma_{y}(x)\sigma_{z}(x)} \exp\left\{-\frac{y^{2}}{2\sigma_{y}(x)^{2}}\right\}$$

$$\times \left\{\exp\left[-\frac{(z-h)^{2}}{2\sigma_{z}(x)^{2}} + \gamma \exp\left[-\frac{(z+h)^{2}}{2\sigma_{z}(x)^{2}}\right]\right\} \begin{array}{c} (grams/cubic meter) \end{array}$$

Where: $\bar{\chi}$ = mean concentration (grams/cubic meters)

Q = emission rate (constant, grams/second)

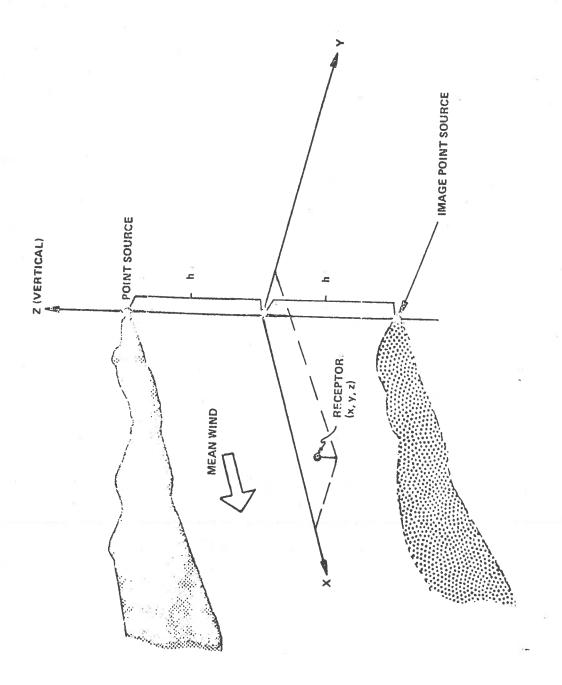


Figure 1. Point Source

h = source height (meters)

 γ = absorption coefficient (γ = 1.0 indicates non-absorbing ground surface)

 $\sigma_{x}(x), \sigma_{z}(x) =$ standard deviations of lateral and vertical relative concentrations distributions, respectively (meters)

In order to apply the above equation to the highway dispersal problem, the functions $\sigma_{_{\mbox{\scriptsize X}}}(x)$ and $\sigma_{_{\mbox{\scriptsize Z}}}(x)$ must be defined. The ESL model utilizes the following functions reported in "Meteorology and Atomic Energy" (Clifford, U.S. Atomic Energy Commission, July 1968):

$$\sigma_{\mathbf{y}}^{\prime}$$
 (x) = $\frac{\sigma_{\theta}}{1.23}$ X $\sigma_{\mathbf{z}}^{\prime}$ (x) = $\frac{\sigma_{\phi}}{1.23}$ X

The σ_{θ} and σ_{φ} parameters can either be assigned by field measurements or the Pasquill Turbulence Classification.

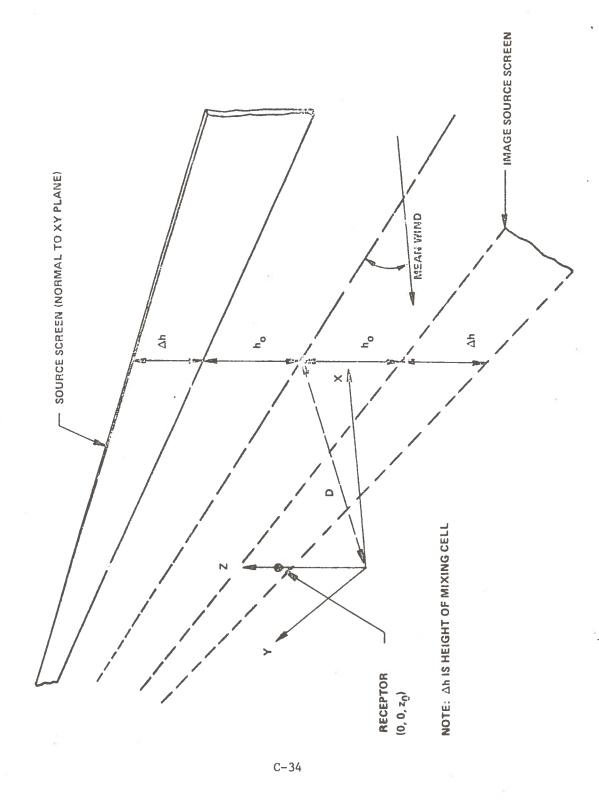
The high-speed highway vehicular traffic generates mechanical turbulence which rapidly disperses vehicular emissions throughout a volume over the roadway surface. In simplest terms the cross section of this volume (or mixing cell) is rectangular in shape with a height Δh and width equal to the roadway. This mixing cell is also assumed to extend along the entire length of the roadway. The vehicular pollutants, then, are assumed to elude from a screen which is the downwind vertical side of the

mixing cell; thus, the screen is located at the downwind edge of the roadway with the height of the mixing cell (Δh) and length of the roadway. For at-grade and elevated roadways, the screen base is placed at the roadway level; however, for cut roadways, the screen base is placed at ground level (but over the downwind . roadway edge). Figure 2 diagrams this geometric configuration. The ESL model is then developed by assuming the vehicular emissions elude uniformly from the screen; therefore, the screen can be considered to consist of an infinite array of point sources. The concentration at a receptor point from each point source is calculated by using the Gaussian equation. Consequently, the sum of concentrations from all these point sources is the concentration from the screen. Mathematically, the summing process reduces to integrating the Gaussian equation over the screen. If the receptor point is close to the roadway, the roadway can be considered infinite in length; then, the integration along the length of the screen can be performed analytically to yield:

$$\bar{\chi} = \int_{h_{0}}^{h_{0} + \Delta h} \sum_{A=z_{0}-h, z_{0}+h} \gamma_{A} \sqrt{\frac{2\pi}{0.661\sigma_{\phi}^{2}D^{2} + 0.661\sigma_{\theta}^{2}A^{2}\cos^{2}\alpha}}$$

$$\times \exp\left[\frac{-A^{2}\sin^{2}\alpha}{2(0.661\sigma_{\phi}^{2}D^{2} + 0.661\sigma_{\theta}^{2}A^{2}\cos^{2}\alpha)}\right]$$

$$\times \left(1 + \operatorname{erf}\left[\frac{0.813\sigma_{\phi} D \tan \alpha}{\sqrt{2}0.813\sigma_{\theta}(0.661\sigma_{\phi}^{2}D^{2} + 0.661\sigma_{\theta}^{2}A^{2}\cos^{2}\alpha)}\right]\right) dh$$



Where:

q = emissions per unit length (grams per meter per second) α = angle between the wind direction and roadway length γ_A = 1 if A = Z_O -h or γ_A = γ if A = Z_O +h

erf (Z) =
$$\frac{2}{\sqrt{\pi}}$$
 $\int_{0}^{Z} e^{-t^2} dt$, the standard error function

In general, the vertical integration (between h_{o} and h_{o} + Δh) is performed numerically. However, for two special cases of parameters, an analytical solution can be easily developed.

In the first case, the term $.661\sigma_0^2\cos^2\alpha$ in the above equation can be neglected because either α is sufficiently close to $\pi/2$ or $A^2\sigma_\theta^2$ is small compared to $\sigma_\phi^2D^2$. Then the above equation is analytically integrated to yield:

$$\overline{\chi} = \frac{q}{2\overline{u} \sin \alpha} \left[1 + erf\left(\frac{\tan \alpha}{0.813\sqrt{2}\sigma_{\theta}}\right) \right] \left\{ F\left[\frac{(h_0 + \Delta h - z_0) \sin \alpha}{0.813\sigma_{\phi}}\right] \right\}$$

$$-F\left[\frac{(h_{O}-z_{O})\sin\alpha}{0.813\sigma_{\phi}}\right]+\gamma F\left[\frac{(h_{O}+\Delta h+z_{O})\sin\alpha}{0.813\sigma_{\phi}}\right]-\gamma F\left[\frac{(h_{O}+z_{O})}{0.813\sigma_{\phi}}\right]$$

Where:

$$F(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{t} e^{-s^2/2} ds, \text{ the standard normal cumulative distribution}$$

In the second case if $\alpha = 0$, the equation is also analytically integrable to yield:

$$\overline{\chi} = \frac{q}{2\sqrt{2\pi u}} \left[\ln \left(\frac{h_o + \Delta h - z_o + \sqrt{(h_o + \Delta h - z_o)^2 + 0.661\sigma_\phi^2 D^2}}{h_o - z_o + \sqrt{(h_o - z_o)^2 + 0.661\sigma_\phi^2 D^2}} \right] + \gamma \ln \left(\frac{h_o + \Delta h + z_o + \sqrt{(h_o + \Delta h + z_o)^2 + 0.661\sigma_\phi^2 D^2}}{h_o + z_o + \sqrt{(h_o + \Delta h + z_o)^2 + 0.661\sigma_\phi^2 D^2}} \right) \right]$$

Application of the Model.

In order to apply the model, it is necessary to define the following parameters for one of the three above mathematical equations:

traffic related: q -- emissions per unit length per unit time

Δh -- height or mixing cell

roadway-related:

h -- distance between the roadway surface and the ground

pollutant-related: γ -- absorption coefficient

meteorological: \bar{u} -- wind speed

 α -- angle between the wind direction and roadway

 $\sigma_{\theta}, \sigma_{\phi}$ -- horizontal and vertical wind direction variancies, respectively

ESL has applied the model to predict air pollution dispersal from highways in over six states geographically distributed throughout the nation. What follows is the methodology developed and employed to calculate the above parameters. For some of these parameters, in particular Δh , the assigned value is based entirely on experimental field data. These parameters have been found to vary among the various locations; however, in the absence of local data, typical values can be assigned.

Regarding traffic related parameters, the value of q is calculated by using the methodology described in the U.S.E.P.A.'s publication: "Compilation of Air Pollutant Emission Factors" (AP-42). The value of Δh has been determined by regression analyses utilizing field data to be approximately 10 feet; thus, this value is inserted in the absence of local data.

Regarding the roadway related parameter, the value of $h_{\rm O}$ is simply taken as the difference between the road height and the mean ground level for elevated and at grade roadways. For cuts, $h_{\rm O}$ is set equal to zero (i.e., the emitting screen is placed at ground level above the roadway surface).

Regarding the pollutant-related parameter, the value of γ for carbon monoxide is taken as unity. This assignment has been extensively verified by field tests. Since carbon-monoxide is essentially unreactive the absence of absorption is expected. Because the chemical reactions of other gaseous pollutants are relatively slow, in previous studies, ESL has assumed that the unity assignment would apply to hydrocarbons and total nitrogen oxides. However, in the case of particulates, the value γ has been observed to be approximately 0.5; thus, this value is applied in the absence of other data.

Regarding the meteorological parameters, there are two types of meteorological situations which must be addressed:

- (1) A meteorological situation in which there is a definite wind speed, wind direction and Pasquill Turbulence Class.
- (2) A meteorological situation which is simply described as a calm (i.e., there is no definite wind, and existing air movements are erratic and slow).

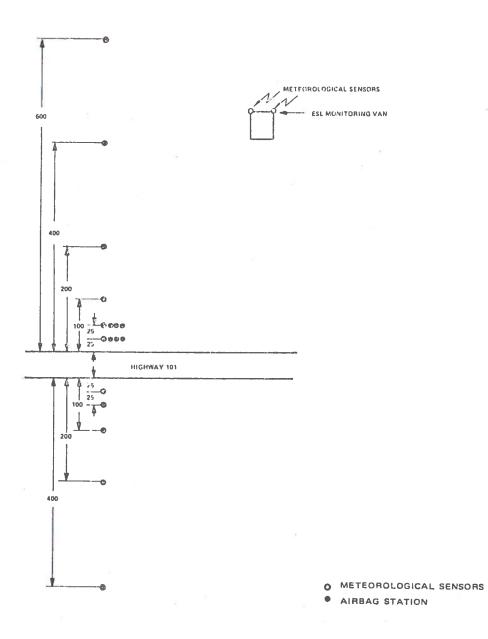
Assignment of meteorological parameters in the first situation is relatively straight forward. The actual (or assumed) wind speed (\bar{u}) and direction (α) are applied. Using the methodology in the "Workbook of Atmospheric Dispersion Estimates" Bruce Turner 1970, the actual (or assumed) Pasquill Turbulence Class is employed to assign values for σ_{θ} and σ_{ϕ} .

Assignment of the meteorological parameters in second situation relies on experimental field data. From validation data which was acquired under very calm meteorological conditions at the bottom of a valley, a regression analysis indicates that the following parameters, when they are substituted into the model equations, accurately calculate the concentrations: $\bar{u}=0.7$ meters per second, $\gamma=90^{\circ}$, and σ_{θ} and σ_{φ} correspond to the Pasquill Turbulence Class C.

Validation Data.

Under contract to various highway departments throughout the nation, ESL has acquired extensive sets of carbon monoxide and particulate (especially lead) validation data. The majority of this data was acquired using multiple air bags which were simultaneously and automatically filled over a specified time period; during this time period, meteorological and traffic data were also concurrently acquired. The contents of the air bags were analyzed for their carbon monoxide concentration using a gas chromatograph.

Figure 3 shows a typical arrangement of the equipment employed for the measurement of carbon monoxide levels near the roadway. Figures 4 and 5 are photographs of this particular experimental site. Normally such air bags were filled using "Star" Aquarium pumps with a needle valve and bleeder in the output from the pump to the air bag as shown in Figure 6. With different adjustments of the valve, the air bags can be filled in as little as 5 minutes or as long as two hours. Aluminized "Scotch-Pak" bags were used to collect the atmospheric samples.



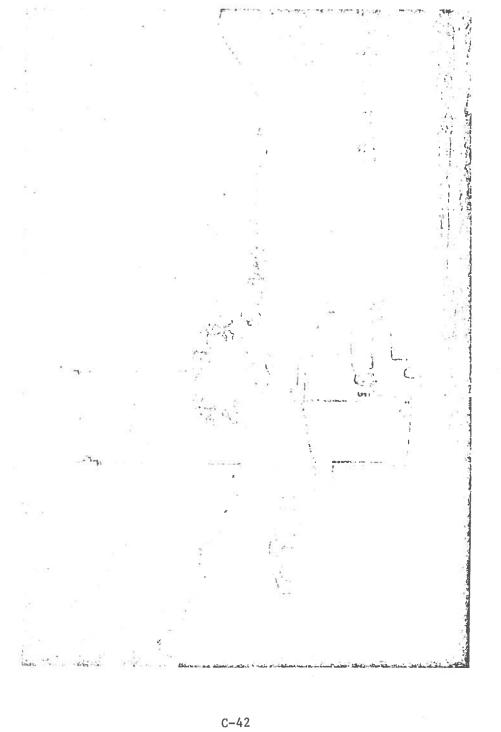
NOTE: DISTANCES ARE IN FEET

Figure 3. Diagram of a Typical Open Roadway Validation Experiment

These remotely controlled air bag samplers and hivols were used in the Field Experiment in Cloverdale, California by Highway 101. NOTE:

Photograph of Typical Validation Experiment

Figure 4.



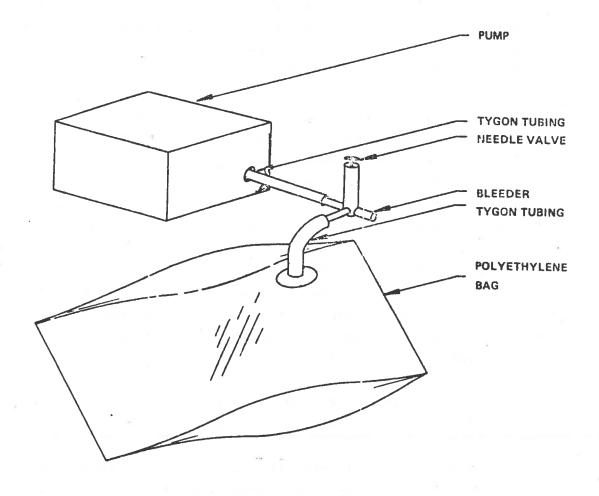
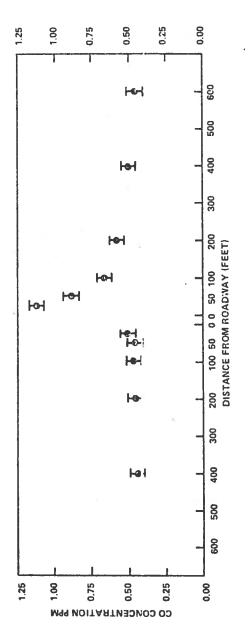


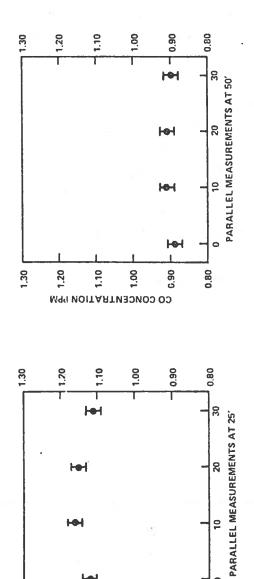
Figure 6. Diagram of Air Bag Pump

Most validation sets of air bags which have been employed in model validation and calibration efforts were filled in approximately 60 minutes. This time period was selected in order to assure that the variance in the concentration measurement from statistical fluctuations in atmospheric dispersal characteristics and traffic emissions would be small compared to the mean values. The good agreement observed between similar data sets and the nearly identical concentrations measured from air bags located at the same distance from the roadway indicate that these conditions were achieved.

The array of air bags was designed to measure several critical parameters. Air bags were located at distances up to 600 feet from the roadway. Bags were located on both sides of the roadway in order to obtain a good estimate of "upwind" background levels and to examine the levels on both sides of the roadway during calm or nearly parallel winds. In addition, several bags were located at the same distance from the roadway but displaced from each other by 3 meters (10 feet) parallel to the roadway. The purpose of these bags is to determine the reliability and variance associated with the measurements. Also, such measurements provide a test on the uniformity of levels parallel to the roadway.

Figure 7 describes a sample of a set of validation data. The error bars describe plus and minus one standard deviation of variance associated with the bags parallel to the roadway. As can be seen in the figure, in this particular situation concentrations measured were less than or equal to 1 mg/m^3 (or 1 ppm) of carbon monoxide. A gas chromatograph was used to







0.80

1.30

accurately measure these low concentrations. The gas chromatograph (Beckman Model 6800) measured relative concentrations which were accurate to within 2%. The absolute accuracy was limited to the accuracy of calibration gases. Concurrently with the air bag collection, Hi Vols-were operated at various distances from the roadway to collect particulate validation data.

Least-squares analyses utilizing validation data obtained in this fashion were performed in order to determine the values of the empirical parameters (in particular Δh and γ) and validate the ability of the model to accurately calculate pollutant concentrations near the highway from highway traffic. Figures 8, 9 and 10 are typical comparisons of the model calculations and the measured concentrations for the three major roadway geometric configurations. As seen in these figures, the ESL model accurately calculates concentrations of air pollutants near the roadway.

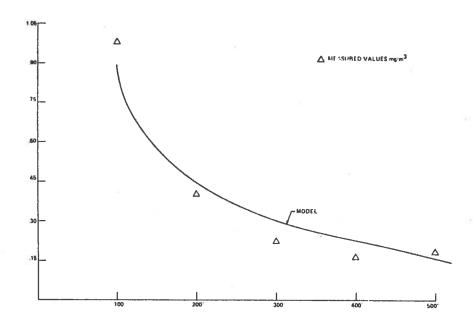


Figure 8. In Cut Highway Configuration

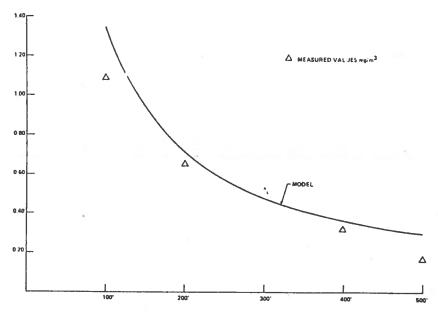


Figure 9. At Grade Highway Configuration

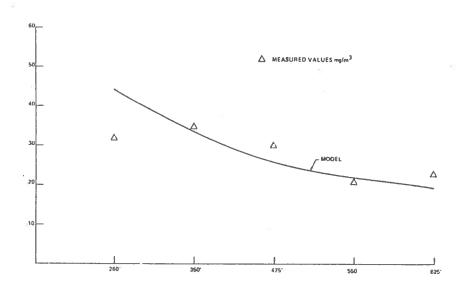


Figure 10. Elevated Highway Configuration

C.6 GENERAL ELECTRIC (GE)

The G.E. Model

The model was developed by the General Electric

Company under a contract with the City of New York.** The purpose of this contract was to produce a model for predicting air quality (i.e. CO concentrations) in the immediate vicinity of various urban roadway configurations. The configurations studied were the following:

Covered on top, open on one side
Long tunnel, ventilated
Shallow Cut
Short tunnel, unventilated
Deep cut
Grade road
Cantilever cover
Viaduct
City street
Intermittent covered span

The G.E. Model assumes that the decrease in concentration of CO with height can be represented by the following exponential relationship:

$$C = \frac{MN}{W(aD+V)} e^{-az}$$
 (1)

where

M = pollutant emissions in mass per vehicle mile

 \dot{N} = traffic flow rate in vehicles per hour

a = a constant found to be .015 to .025 ft.⁻¹

W = width of the roadway

^{**}Study of Air Pollution Aspects of Various Roadway Configurations, Final Report, New York City Contract No. 209624, General Electric Company, September 1971.

D = diffusion coefficient

V = wind_velocity

z = height above vehicle exhaust plane

C = concentration of CO

If z is replaced by the radial distance ρ then (1) becomes:

$$C = CO_{x} e^{-ap}$$
 (2)

where

$$CO_X = \frac{MN}{W(aD+V)}$$

which is the concentration resulting from the xth line source.

ρ = the radial distance between the source and the receptor (the point at which the concentration is calculated).

This model was further refined by defining a vehicular pollution factor ϕ where:

$$\phi = \frac{CO_X}{\dot{N}} = \frac{M}{W(aD+V)}$$
 (3)

For eight of the ten highway configurations listed above (i.e. all except the tunnels), G.E. discovered that there is a strong linear relationship between ϕ and traffic speed. The regression relationship for the year 1971 was found to be:

$$\phi_i = \left[-0.51 \, T_i + 26.9\right] \times 10^{-3} \, \frac{\text{ppm-hr}}{\text{vehicle}}$$
 (4)

for 15 mph \leq T \leq 49 mph

 T_i = average traffic speed in lane i.

The total CO concentration at receptor R, ${\rm CO}_{\rm R}$, is then obtained by summing the contribution of the S road lanes:

$$CO_{R} = \sum_{i=1}^{S} \phi_{i} \dot{N}_{i} e^{-a\rho_{i}R}$$
 (5)

C.7 INTERA (INT)

TSC DISPERSION MODEL VALIDATION TESTS

Summary of Technical Approach

- (1) Turbulent diffusivities used were consistent with the Pasquill-Gifford stability classes. That is, we have shown¹ that the Fickian type diffusivity model can give results virtually identical to the Gaussian models provided both the eddy diffusivities and the wind speed are made functions of height within the boundary layer. These values which we have previously found consistent with the Pasquill-Gifford stabilities were used in this study. To accommodate a seventh stability class, we have extrapolated the diffusivities to provide a more stable class than Pasquill-F.
- (2) Emission levels for the vehicles were assumed to be 6 x 10⁻³ ft³ of CO/sec/vehicle/ft of roadway. This is equivalent to a release of 37.5 gm of CO/mile for each vehicle. Since no information was provided on the relative traffic flows per lane, we have assumed an equal distribution per lane. Our release in the vertical direction was between ground level and 9 feet uniformly. This distribution in the vertical reflects our opinion that the warm roadway and thermal buoyancy of the exhaust in addition to the eddy motions caused by vehicular travel create an effective vertical release.
- (3) All cases were calculated as two-dimensional. Calder² has shown that utilizing the wind component normal to the roadway along with the actual downwind distance from the roadway to the receptor (measured along the wind direction) is in good agreement with the exact integration. For angles up to 75° from perpendicular, the agreement for a Gaussian model was exact to three decimals. Moreover, steady-state Gaussian models are a poor approximation to the parallel wind case since the effect of both transients and finite length road segments are important.

Since transients and finite road segments are important, we have omitted in our analysis any case in which the wind direction was within $\pm~10^{\circ}$ from parallel to the roadway; not because these cases could not be run, but rather because the along roadway segment lengths were unknown. At site 11, eight of the 160 cases were omitted. These were cases 19, 41, 88, 89, 99, 100, 101, and 109. At site 14, one of the 90 cases (case 10) was omitted. At site 15, none of the 25 cases was omitted.

- (4) At site 15 (with an elevated roadway), preliminary calculations indicated the flow remained essentially parallel to the elevated section. As a consequence, the test cases were calculated using this assumption.
- (5) Initially, we examined in detail the calibration data. Based upon a cursory examination of the data, it appeared that the measured concentration buildups would not correlate well with source strength. That is, the concentration increase from the roadway did not appear to correlate well with the number of vehicles per hour given that stability class, wind speed, wind direction and vehicle speed were essentially constant. As a consequence of this cursory examination, we did a regression analysis of the calibration runs. To allow linear regression analysis, the variables were transgenerated. As an example, one of the regression analyses examined the equation:

$$C_i = \alpha N_{i/U_i} e^{-\beta Z_i^2}$$

where C_i = the concentration increase downwind over upwind

N; = the number of vehicles/hr.

 $U_i = wind speed$

 Z_{i} = the elevation of a receptor

 $\alpha, \beta = regression constants$

and i = individual data point

The above equation obviously ignores effects of atmospheric stability and wind direction; however, other regression runs included these variables as well.

This regression analyses indicated that for either site 11 or site 14, the calibration data concentration increases, although correlated with the source rate (number of vehicles), showed a general inverse relationship. That is, the greater the number of vehicles, the lower the concentration increase. Of course, the number of samples at each site was small and often part of these were deleted to avoid the problem of parallel winds discussed earlier. Still, this finding disturbed us sufficiently that we contacted TSC about the problem.

TSC examined the test data and found that the complete set of data did correlate with the number of vehicles. As a consequence, we have virtually ignored the calibration data and provided predictions based upon our limited experience in traffic modeling.

What we had hoped to back out of the calibration data was the most representative vertical distribution of carbon monoxide emissions above the roadway. Because of the limitations in the calibration data discussed above, this was not possible.

Instead, our distribution was consistent with our previous experience from a traffic validation study conducted by EPA. This experience is obviously somewhat limited.

Description of Model

General

The model used is a numerical solution of the three-dimensional material balances for both pollutant transport and for the air stream. The pollutant transport equation includes advection and turbulent diffusion. The turbulent diffusion is characterized by a Fickian approach with spatially dependent properties. In particular, the turbulent diffusivities are made a function of height within the boundary layer. The wind calculation, though based upon a modified potential flow, allows the horizontal wind to vary with height. The modified potential flow allows (1) inviscid potential flow at high elevations and (2) empirical height-dependent coefficients which account for surface friction (viscous effects) within the boundary layer.

Application to Traffic Problem

The user must specify a set of three-dimensional grid blocks. Variable grid spacing allows the user sufficient flexibility to include adequate description of the emission source distribution. In the case of application to traffic problems, the emission source generally takes the form of connected finite-length line segments.

In the validation tests, the receptor locations were relatively close to the roadway. Moreover, no line segment specification of roadway path was provided so that we treated this application as an infinite-length line segment. Calder² has shown that a good approximation for a wind oblique to a line source can be determined from the perpendicular wind line source solution. This takes the form

$$\frac{C \sim \frac{\psi(x/\cos\theta)}{\cos\theta}}$$

 ψ = the solution for a perpendicular wind

 θ = the wind angle measured from perpendicular

This was the concept used in the present study allowing the calculations to be two-dimensional instead of three.

The program calculation proceeds by specifying the grid, line (area) source locations, background concentration levels, and receptor locations as if the wind were going to be perpendicular to the roadway. For any specified wind direction, the program then automatically adjusts the grid block sizes in the x-direction by dividing by cose. The wind speed is also adjusted to give the perpendicular component (totally equivalent to dividing the perpendicular line source solution by cose as specified in Calder's paper). The program then proceeds with a normal two-dimensional, x-z, finite difference calculation of wind perpendicular to a single or series of line (area) sources.

Program Input

The user must specify a number of input variables. The physical meaning and a brief description of these variables is summarized below:

- (1) Program control information including the number of grid blocks in each of three directions (for 2-D one is permissable), output desired, the number of source blocks, and other similar data;
- (2) Source location and magnitude specification including the number of traffic lanes, their location in the grid, the vertical blocks above the roadway through which this emission is to be distributed and the relative emission weighting factors for the vertical distribution for each lane;
- (3) The vertical distribution of the background concentrations which flow across the x = 0 face of the grid;
- (4) The definition of grid block sizes (normally one x-grid block is used to describe each traffic lane) in each coordinate direction;
- (5) Wind direction and speed, atmospheric stability, mixing layer height if vertical diffusion is to be limited; and
- (6) Receptor x, y, z coordinates

Program Output

The user has considerable control in the kind of output he desires to see. The output which always is printed includes the control information, the source locations and strengths, the block sizes, the wind direction and speed, and the receptor concentrations. Optional output includes:

- (1) concentrations in each grid block,
- (2) printer contour maps of the concentrations, and
- (3) wind velocity output for each coordinate direction.

Model Equations

The attached abstract includes a brief description of the equations and method of solution used in the finite difference model.

References

- Lantz, R.B., Coats, K.H., and Kloepfer, C.V.; "A Three-Dimensional Numberical Model for Calculating the Spread and Dillution of Air Pollutants", Proceedings Air Pollution, Turbulence, and Diffusion Symposium, December, 1971.
- Calder, K.E.; "On Estimating Air Pollution Concentrations from a Highway in an Oblique Wind", Atmospheric Environment 7, 1973.

ATTACHMENT I

AIR QUALITY MODEL

3.1	WIND CALCULATION CONSIDERING TOPOGRAPHY
densi	Material balance on the flowing air stream, assuming constant ity, gives
	$\nabla \cdot \overline{U} = 0$ (1)
where	3 ·
	T = the time-averaged air velocity vector, consisting of components u, v and w in the x, y and z directions, respectively.
If a	velocity potential defined by
	$\overline{\overline{U}} = \nabla \phi$ (2)
is in	stroduced into Equation (1) Laplaces' equation is obtained:
	$\nabla^2 \dot{\phi} = 0 (3)$
Solution potential form the grand mand in looked behaves mand mand mand the solution of the so	The assumption that the fluid motion is irrotational is sined in the definition of potential given by Equation (2). Sion of Equation (3) for boundary conditions of constant atial in the vertical direction and no terrain feature results orizontal velocities which do not vary with height. Near ground surface, however, air viscosity becomes important assurement of turbulent flow over a flat plate are found to vary original constant or power law fashion. To account for this known vior, the definition of velocity potential in Equation (2) and defined to include an empirical resistance "flow coefficient", even by
	$\overline{U} = K \nabla \phi$ (4)
where	K has components Kx, Ky, Kz.
respo terra law o can b	As a consequence, over flat terrain, the horizontal velo- es will have the same variation with height as do the cor- onding flow coefficients in that direction. Over uneven ein, vertical and crosswind flow will modify this power or logarithmic variation. Additionally, these coefficients be varied spatially to indicate different amounts of surface eness. Substituting Equation (4) into Equation (1) gives

These empirical resistance flow coefficients do have physical significance. In laminar steady flow over a flat plate, the horizontal velocity is proportional to a function of height (a height squared relationship) multiplied by the fluid potential defined by $p + \rho g Z$, where p = pressure, $\rho = fluid density$, g = the gravitational constant and <math>Z = vertical height. If a turbulent eddy viscosity is defined analogous to the Newtonian molecular viscosity, the same type of expression can be derived; however, a different functionality with vertical distance from the ground surface should be expected. This is our concept for the horizontal flow coefficients, K_X and K_Y . These coefficients are normally taken as power law functions of height as follows:

$$K_{X}$$
, $K_{Y} = \begin{cases} (Z/Z_{O})^{\alpha} & \text{for } Z < Z_{O} \\ \text{unity} & \text{for } Z > Z_{O} \end{cases}$ (6)

The vertical coefficient, other than for flow vertically along a cliff, should be only slightly affected by the viscous friction of the ground surface. As a consequence, the vertical variation of this resistance coefficient, $K_{\rm Z}$, realistically reflects the density variation with height. For neutral conditions the adiabatic lapse rate gives $d\rho/dZ=0$ and the coefficient, $K_{\rm Z}$, would be approximately unity. For stable conditions, there is a severe restriction to vertical flow and $K_{\rm Z}$ should be significantly less than unity. Our approach has been to assume $K_{\rm Z}$ is constant but varies with atmospheric stability from roughly 0.01 for stable conditions up to 1.0 for unstable conditions.

Solution of Equation (5) for the potential, ϕ , along with Equation (4) gives the three-dimensional velocity field U. The boundary condition used for Equation (5) is that the wind is one-dimensional along the external boundaries. That is, u is specified and v and w are zero. The horizontal velocity at the boundary can, of course, be variable with height. No flow boundaries representing terrain are created by setting the appropriate direction flow coefficients to zero.

Formulation of the air flow in terms of a modified velocity potential represents a significant simplification. Neglected in such an approach are such factors as (1) the change in wind direction with increasing elevation (Ekman spiral), (2) formation of eddies on the downwind side of obstacles to flow and (3) thermal or any density instability which can cause vortices in the flow.

Our model for describing wind flow over irregular terrain features has been kept simple for two reasons. First, we did not want to consume a disproportionate share of computer time in solving the wind flow problem compared to that required for the turbulent diffusion solution. Second, the mathematical description

of individual eddies downstream from obstacles in the flow is probably not essential to the pollutant dilution problem. In fact, refinement in the grid to adequately compute eddy formation will generally be impractical for realistic terrain problems. In a gross sense, the increased dispersion of pollutant due to eddy formation can be approximated by increasing the eddy diffusivity downstream of obstacles. In our model, we have made the diffusivities dependent on velocity, and thus an increase in diffusion occurs automatically as the flow progresses around an obstacle.

The finite difference representation used for Equation (5) was

$$\Delta (T\Delta \phi)_{ijk} = 0 \qquad (7)$$

where T is the transmissibility at any point, defined as follows:

$$\begin{split} & \Lambda \left(\mathrm{T} \Delta \varphi \right) \ = \ \Delta_{\mathrm{X}} \left(\mathrm{T}_{\mathrm{X}} \ \Delta_{\mathrm{X}} \ \varphi \right) \ + \ \Delta_{\mathrm{y}} \left(\mathrm{T}_{\mathrm{y}} \ \Delta_{\mathrm{y}} \ \varphi \right) \ + \ \Delta_{\mathrm{z}} \left(\mathrm{T}_{\mathrm{z}} \ \Delta_{\mathrm{z}} \ \varphi \right) \\ & \Delta_{\mathrm{X}} \left(\mathrm{T}_{\mathrm{X}} \ \Delta_{\mathrm{X}} \ \varphi \right) \ = \ \mathrm{T}_{\mathrm{i} + \mathrm{i}_{\mathrm{z}}} \left(\varphi_{\mathrm{i} + \mathrm{l}} \ - \ \varphi_{\mathrm{i}} \right)_{\mathrm{j} \mathrm{k}} \ - \ \mathrm{T}_{\mathrm{i} - \mathrm{i}_{\mathrm{z}}} \left(\varphi_{\mathrm{i}} \ - \ \varphi_{\mathrm{i} - \mathrm{l}} \right)_{\mathrm{j} \mathrm{k}} \\ & \mathrm{T}_{\mathrm{i} + \mathrm{i}_{\mathrm{z}}}, \mathrm{j} \mathrm{k} \ = \ \left(\mathrm{K}_{\mathrm{X}} \ \Delta \mathrm{y} \ \Delta \mathrm{z} / \Delta \mathrm{x} \right)_{\mathrm{i} + \mathrm{i}_{\mathrm{z}}}, \mathrm{j} \mathrm{k} \end{split}$$

Equation (7) is solved by the line successive over-relaxation (LSOR) method. This is an iterative procedure which develops the steady flow solution through a reduction of the coefficient matrix to tridiagonal by calculating the vertical direction potentials at the new iterate while the others are at known iterate levels. Iteration proceeds until the material balance error is acceptable.

Convergence of the iterative procedure can be accelerated by the choice of a "good" iteration parameter. Theory has been adequately developed for estimating an optimum iteration parameter for the LSOR procedure. This determination depends upon estimating the spectral radius of the Gauss-Seidel matrix. This procedure has been included in the program. As a consequence the program makes a few iterations (5 or more should be used) on the terrain problem specified with slightly different boundary conditions. Based upon the maximum change in potential during iterations of this modified problem an estimate of the optimum parameter can be calculated. This parameter is then used in iterations on the actual wind flow problems.

3.2 TURBULENT DIFFUSION

Material balance on the pollutant flowing in the air stream with velocity field, \overline{u} , defined in the previous sections gives:

$$\nabla \cdot E\nabla C - \overline{U} \cdot \nabla C + r = \frac{\partial C}{\partial t} + q_S + q_A \dots (8)$$

where:

C = pollutant concentration, lbs pollutant/lb air

E = eddy diffusivity with components E_X, E_V, and E_Z in ft.²/sec.

r = rate of disappearance of pollutant due to reaction, lb
pollutant/sec/lb air

qs= pollutant source rate, lbs pollutant/sec./lbs air

qa= pollutant ground adsorption rate, lbs pollutant/sec/lb air

t = time, sec.

The rate of disappearance of pollutant by chemical reaction, r, is assumed to be first-order and thus is proportional to the concentration. The pollutant source rate, q_s , is the pollutant mass source rate per unit volume of the total emission, divided by the air density. The ground adsorption rate, q_a , is the mass rate of pollutant absorbed (or adsorbed) at ground level per unit surface area multiplied by the specific surface of the ground and divided by the air density.

Equation (8) can be solved once the velocity field, $\overline{\mathbf{U}}$, and the boundary conditions are specified. Calculation of the velocity profile is discussed in the previous section. Boundary conditions for diffusion are that the flux normal to the ground surface, at the upper and side boundaries is zero. The upper boundary can represent a temperature inversion if desired.

The finite-difference approximation used for Equation (8) is of the form:

$$(\Delta T\Delta C)_{ijk,n+1} - \Delta y (vA_yC)_{ijk,n+1} - \Delta_z (vA_zC)_{ijk,n+1} + V_{ijk}(q_{s,ijk} - \frac{\ln 2}{\tau} C_{ijk,n+1}) = \Delta_z (uA_zC)_{ijk,n+1} + \frac{1}{\Delta \tau} (V_{ijk} + \frac{A_z\Delta C_s}{\rho\Delta C})$$

$$(C_{ijk,n+1} - C_{ijk,n}) \qquad (9)$$

where:

$$\Delta \left(\text{T}\Delta \text{C} \right) \; = \; \Delta_{\text{X}} \left(\text{T}_{\text{X}} \Delta_{\text{X}} \text{C} \right) \; + \; \Delta_{\text{Y}} \left(\text{T}_{\text{Y}} \Delta_{\text{Y}} \text{C} \right) \; + \; \Delta_{\text{Z}} \left(\text{T}_{\text{Z}} \Delta_{\text{Z}} \text{C} \right)$$

A = cross sectional area, ft.²

$$\Delta_{y}(T_{y}\Delta_{y}C) = T_{ij+\frac{1}{2}\sqrt{k}}(C_{j+1} - C_{j})_{ik} - T_{ij-\frac{1}{2}\sqrt{k}}(C_{j} - C_{j-1})_{ik}$$

$$T_{ij+\frac{1}{2},k} = (E_y \Delta x \Delta z / \Delta y)_{ij+\frac{1}{2},k}$$

$$\Delta_{\mathbf{y}}(\mathbf{v}\mathbf{A}_{\mathbf{y}}\mathbf{C}) = (\mathbf{v}\Delta\mathbf{x}\Delta\mathbf{z})_{\mathbf{j}+\frac{1}{2}}\left[\alpha\mathbf{C}_{\mathbf{j}} + (1-\alpha)\mathbf{C}_{\mathbf{j}+\mathbf{1}}\right] - (\mathbf{v}\Delta\mathbf{x}\Delta\mathbf{z})_{\mathbf{j}-\frac{1}{2}}\left[\alpha\mathbf{C}_{\mathbf{j}-\mathbf{1}} + (1-\alpha)\mathbf{C}_{\mathbf{j}+\mathbf{1}}\right]$$

$$(1 - \alpha)C_j$$

 $V_{ijk} = block volume (\Delta x \Delta y \Delta z)_{ijk}$

 $\frac{\Delta C_{\rm q}}{\rho \Delta C}$ = slcpe of the adsorption isotherm, ft³/ft²

C_s = mass pollutant/unit area, lb/ft²

 $\rho = air density, lb/ft^3$

i,j,k = x,y,z indices

n = the time level index

 Δx , Δy , Δz , $\Delta t = x$, y, z, and the time increments

 τ = the reaction half-life

 α = weighting parameter

3.3 TRUNCATION ERROR

The weighting parameter, α , makes possible several different choices of space difference approximations to the first order convection derivatives. In the program, we have selected a first order correct upstream weighting (if $v_{j+\frac{1}{2}}$ is negative, $\alpha=0$; if $v_{j+\frac{1}{2}}$ is positive, $\alpha=1$). A second order correct central difference ($\alpha=0.5$) could have been used. However, the central difference gives rise to a damped oscillation if the eddy diffusivity E is not greater than u4x/2. The first order correct procedure does not cause this oscillation but has the disadvantage that it introduces a numerical diffusivity equal to u4x/2 (Reference 13). Depending upon the block sizes used this numerical diffusivity could dominate the desired eddy diffusion coefficient.

Fortunately plume dispersion is quite insensitive to the diffusion which occurs along the plume centerline. As an illustration, the Gaussian plume models do not even contain a coefficient for mixing in the direction of flow. We have made calculations with substantial variations in the diffusion levels in the downwind direction and verified the minimal importance of this coefficient. Velocities in the crosswind and vertical directions are generally much smaller and thus the space truncation error which is proportional to velocity is ordinarily negligible.

Time truncation error can also be important. The first order time derivative approximation results in an apparent diffusivity equal to $\hat{u}^2\Delta t/2$. If instantaneous releases of pollutant were important (for example a few minute tracer release), small time steps would be required to assure a negligible time truncation

error. For the most part, the problems of interest are continuous releases with wind changes occurring on the order of hours. Under these circumstances, the concentrations within the region 5-10 miles downwind from the stacks is near steady-state. Time truncation for steady state problems is not present, thus the calculated concentrations for these cases is accurate.

Alternative approaches such as Lagrangian methods (Reference 14) and variational methods (Reference 15) have been used to minimize truncation errors. However, our experience comparing the numerical model with analytical solutions indicates truncation error will not be an important limitation for the majority of the problems of interest.

C.8 KAMAN SCIENCES CORPORATION (KAM)

KAMAN SCIENCES CORPORATION LINE SOURCE MODEL VALIDATION

INTRODUCTION

The Kaman Sciences Corporation air pollution dispersion model used in this study is Gaussian and can accommodate point, area, and line sources at arbitrary effective heights, and receptors at arbitrary heights. It calculates concentrations of CO, HC, NO_X, SO₂, and particulates. Used here it operated in a mode which excluded point and area sources and all pollutants except CO. The program is written in FORTRAN IV and incorporates unique features which reduce running time significantly below that of similar models.

The KSC Line Source Model was not originally designed for microscale calculation of pollution concentration. For customary problems, the model is used to calculate annual average pollution concentration in the vicinity of finite length highway sections and point and area sources, using annual frequency of wind within direction, speed, and stability classes. For use on highways only, the model is used to calculate hundreds or thousands of highway sections within a metropolitan for dozens or hundreds of receptor locations, usually arranged in a square grid. To eliminate the occasional co-location of a source and receptor, calculations are not permitted within a parametric distance of a source. The most frequently used distance is 0.05 mile (264 ft). Where a receptor grid point is closer than that distance, alternate calculations at a distance of 0.05 mile perpendicular to the highway in both directions is considered as representative of the vicinity.

Despite the interded end use of the model, there are no mathematical restrictions to prevent its use in small scale calculations, and it has been adapted for calculating concentrations of CO close to elevated, at grade, and depressed highways.

DESCRIPTION

This model simulates a line source by dividing a finite length of highway into N square areas, computing the pollution concentration from each area and summing all N areas.

The dispersion equation used is:

$$x = \frac{2Q}{\sqrt{2\pi}\sigma_z u \left(\frac{2\pi x}{16}\right)} = \exp \left[-\frac{1}{2} \left[\frac{H}{\sigma_z}\right]^2\right]$$
 (1)

where the quantities have the customary meaning. This is equation 5.13 from D. Bruce Turner: Workbook of Atmospheric Dispersion Estimates. The downwind distance, X, in this equation is modified by adding a distance ΔX to simulate in the accepted manner distance from each area to a virtual point source upwind a distance ΔX . This equation also assumes that wind direction is not constant, but equally probable within an arc of $2\pi/16$ radians.

ASSUMPTIONS

Assumptions used in this model are typical of those for Gaussian formulations including no change in wind speed with height, a constant wind field during the averaging time, reflection from the ground, mixing height is accounted for in the standard deviation δ_z , and steady state emission during the averaging time.

MODIFICATIONS

The model was modified to the minimum extent required to run the TSC test problems. Modification included changes to vehicles per hour rather than vehicles per day; a single wind sector, speed, and stability rather than all directions, multiple speeds, and five stabilities. (This program uses only one stable class; classes 5, 6 and 7 are identical.)

An expression to compute emission rate as a function of speed used was:

$$Q = 100 \left(0.4 + \frac{280}{(v+2.4)^2}\right)$$
 (2)

where:

Q = CO emission rate per vehicle mile, g/mi.
v = vehicle speed, mph.

A finite length of highway of 1 km was assumed.

The normal output from the program is concentration in $\mu g/m^3$. This was divided by 1205 to change units to ppm. (This factor assumes standard sea level pressure and 10°C.)

Normal Inputs

- 1. Effective height of emmitter above receptor
- 2. Length of highway section
- 3. Orientation of highway
- 4. Traffic count, vehicles
- 5. Number of square areas per highway section
- 6. Location of source(s)
- 7. Location of receptor(s)
- 8. Annual frequency of wind by speed, direction, stability
- 9. Table of emission rates by highway type for each pollutant
- 10. Output format
- 11. Description of grid for receptors and location of other receptors

Normal Outputs

- 1. Annual average concentration for ground level for each pollutant for each receptor on grid and each receptor not on grid, summed over all sources ug/m³
- 2. Total calculated emissions g/sec
- 3. Total vehicle miles per day

Modified Inputs for This Problem

- 1. Same
- 2. 1 Km
- 3. East-West
- 4. Vehicles per hour
- 5. 81
- 6. X = 0, Y = 0
- 7. Same
- 8. Single speed,
 direction,
 stability
- 9. Function
- 10. Same
- ll. Location
 of receptors

Modified Output for This Problem

1. Print concentration for single receptor, single pollutant

```
INFUT DATA--TSC
  11
                  1075
                           35
                                  5
                                      312
                                                  4.8
                                                         4.5
  11
                   989
                           34
                                      340
                                               1
                                                  6.2
                                                         5.9
                                                               5.5
  11
         3
                   643
                           35
                                      345
                                                  5.7
                                                         5.3
                                                               4.9
  11
                  1739
                           34
                                      314
                                                  6.7
                                                         6.4
                                                               5.8
  5.1
                  1504
                           34
                                  6
                                      351
                                               1
                                                  4.5
                                                         4.2
  11
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11	7	6.4 3.6	3.6
11	8	6.5 1.9	1.6
11	9	4.4	2.3
11	10	7.9 / 5.8	5 . 3
11	11	5.4 4.1	4 • 1
11	1.2	6.3 4.9	4.9
11	13	7.0 6.0	6.0
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11	18	3.2 3.0	3.0
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11	23	5.7 4.9	4.3
11	24	4.3 4.6	4.6
		4.1 3.6	3.6
11	25		3.4
11	20	4.0 3.4	
11	27	7.1 4.5	4.3
11	24	10.4 5.€	5.4
11	29	14.0 8.0	7.7
11	30	8.5 4.2	3.8
11	31	7.3 4.5	4.3
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11	36	7.2 6.4	6.4
11	37	9.5 7.5	7.5
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11	39	8.7 6.0	5.9
1.1	4.0	19.3 10.4	9.8
11	41	4.9 4.3	4.2
11	42	7.1 4.4	4.2
11	43	8.0 5.0	5.0
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11	54		
11	55	4.3 2.3	2.2
11	56	4.5	2.3
11	57	5.2 3.1	3.1
11	5 b	4.4 2.4	2.4
11	59	3.0 2.4	2 • 4
11	60	3.2 2.0	2.0

		-104100	-KSC	
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11	84	7.3	6.8	6.8
11	85	7.6	4.9	4 + 8
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11	88	4 - 1	3.8	3 . 8
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11	120	3.3	2.7	2.5
	7	 	6.01	2.7

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11	1 30	1.9	1.5	1.5
11	1.31	3.9	3.0	3.0
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11	133	3.9	1.9	1.9
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11	139	18.2	4.6	4.5
	140			4.5
11		7 • 8	4.5	
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11	142	6.2	5.3	5.3
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11	144	5.3	4 • 6	4.6
11	145	4.5	3.8	3.8
11	146	34	2.5	2.5
1.1	147	4 + 3	4.0	4.0
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		3.4		
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- 14	1	4.0	3.3	3.3
14	2	5 • 2	3.9	3.8
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				2.9
14	12	5.3	3.2	3.2
14	13	8 + 2	6.4	6 • 4
14	14	5.6	4.1	4 • 0
14	15	3.9	2.6	2.5
14	16	2.8	2.0	2.0
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14	19	5.3	3.9	3.9
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4.1	0.4		CHIPUI		
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14	2?		4.2	3 ⋅ β	3.8
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14	24		3.8	3.1	3.1
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14	29		1.6	1.5	1.5
14	30		1.3	1.9	. 3
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14	به له		3.3	2.8	2.7
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14	53		3.8	2.9	2.8
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14	55	1 192	3.2	8 • 8	2.8
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14	57		4.1	2.9	2.9
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14	68		3.1	2.6	2.6
14	69		2.9		
14	70		7.5	1.8	1.8
14					4.3
14	71 72		4.1	3.0	2.9
14			3.9	3.0	2.9
	73 74	12	6 • 8	4.9	4.9
14			3.0	2.5	2.5
14	75 76		3.5	3.0	3.0
14	76		4.3	3.€	3.5
14	77		4.9	3.6	3.6
14	78		3.4	3.0	3.0
14					
14	7 9 80		3.2 3.9	2.8 3.4	2.7 3.3

		OUTPUT	~-KSC			
14	81	5.8	3.1	3.0		
14	82	6.0	5.2	5.2		
14	83	5.8	3.7	3.7		
14	84	5.5	3.9	3.9		
14	85	6.5	6.2	6.2		
14	86	4.9	3.8	3.8		
14	87	4.1	2.6	2.5		
14	83	3.5	2.8	2 • 8		
14	89	4.2	3.5	3.4		
14	-90	8.1	7 . B	7.8		
15	1	3.0	3.1	3.5	6.0	3.1
15	2	4.0	4.1	10.0	10.0	4 . 1
15	3	2.0	2.1	4.0	5.0	2.1
15	4	7.2	7.3	10.7	13.0	7.3
15	5	6.1	€.1	9.0	9. 3	6.2
15	6	10.0	10.0	10.3	11.0	1.0 + 0
15	7	10.0	. 10.0	10.3	11.0	10.0
15	8	0 • 0	• 0	. 3	1 . C	. 0
15	9	5.0	5.0	5.3	6.0	5.0
15	10	6.0	6.0	6.3	6.5	6.0
15	11	6.0	6.0	6.3	6.5	6.0
15	12	6.1	6.1	8.5	11.0	6.1
15	13	6.0	6.1	9.0	15.0	6.1
15	14	7.0	7.1	9.7	15.0	7.1
15	15	2.0	2.0	2.3	4.0	2.0
15	16	2.0	2.0	2.2	4.0	2.0
15	17	3.0	3.0	3.2	5.0	3.0
15	18	2.0	2.0	2.3	2.5	5.0
.15	. 19	3.0	3.0	3.3	4.0	3.0
15	20	4.0	4.0	4.3	5.0	4 . D
1.5	21	2.1	2.2	24.0	24.0	2.3
15	22	3.i	3.2	23.0	23.0	3.3
15	23	3.1	3.2	20.0	20.0	3.2
15	24	6.1	6.1	11.0	21.0	6.2
.15	25	7.1	7.1	8.9	10.0	7.2

6-76

C.9 LOCKHEED MISSILE AND SPACE COMPANY, INC. (LOG)

LOCKHEED POLLUTION DISPERSION MODEL AND VALIDATION EXPERIMENT RESULTS

Alan W. Ratliff Marcus L. Pearson

1.0 INTRODUCTION

Lockheed's pollution dispersion model was adapted from a general computer program written for the solution of viscous mixing and chemically reacting flows associated with such diverse problem areas as rocket collaint plumes and chemical laser cavities. The program is written in FORTRAR IV language and is well documented (Ref. 1). The program's generality permits easy application to atmospheric dispersion problems.

2.0 GENERAL DESCRIPTION

This model is based on a computer program originally written to solve viscous reacting flows with parallel mixing between two or more discimilar streams at constant lateral pressure. The program allows any chemical or vibrational energy exchange reaction mechanism to be prescribed as input data as long as thermodynamic properties and associated rate constants for the reactions are available for all participating species. Transport properties are handled in terms of constant Prantil and Lewis numbers in constantion with a variety of viscosity options which include models for both laminar and turbulent flows. The general formulation of the basic program will be outlined first, then a description of the adaptation of the code to the dispersion problem will be addressed.

Assuming constant lateral pressure, which climinates the lateral momentum equation, the following set of conservation equations are solved simultaneously.

Continuity:

$$\frac{\partial}{\partial \mathbf{x}} (\rho \mathbf{u}) + \frac{\partial}{\partial \mathbf{y}} (\rho \mathbf{v}) = 0 \tag{2.1}$$

Momenturn:

$$u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{dp}{dx} + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right)$$
 (2.2)

Species:

$$\rho u \frac{\partial F_{i}}{\partial x} + \rho v \frac{\partial F_{i}}{\partial y} = \frac{\partial}{\partial y} \left(\frac{Le}{Pr} \mu \frac{\partial F_{i}}{\partial y} \right) + \dot{w}_{i}$$
 (2.3)

Energy:

$$\rho c_{p} \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = u \frac{dp}{dx} - \sum_{i=1}^{NS} h_{i} \dot{w}_{i} + \frac{\partial}{\partial y} \left(\frac{\mu}{Pr} c_{p} \frac{\partial T}{\partial y} \right) + \mu \left[\left(\frac{\partial u}{\partial y} \right)^{2} + \frac{Lc}{Pr} \left(\frac{\partial T}{\partial y} \right) \sum_{i=1}^{NS} c_{p_{i}} \frac{\partial F_{i}}{\partial y} \right]$$

$$(2.4)$$

State:

$$p = \rho R T \sum_{i} F_{i} \frac{\rho R T}{W}$$
 (2.5)

Assuming planar two-dimensional flow, the following initial and boundary conditions apply.

$$x = 0$$
: $u = u(y)$, $T = T(y)$, $F_i = F_i(y)$
 $y = y_0$, $y = y_{max}$:
 $\frac{\partial u}{\partial y} = \frac{\partial T}{\partial y} = \frac{\partial F_i}{\partial y} = 0$ (2.6)

6 Transformation to Stream Function Coordinates

The solution of the governing equations is considerably facilitated by transforming them from the physical x,y-plane into an x,\psi-plane. This transformation (von Mises) is chosen to satisfy the global centinuity equation. Accordingly, the following definitions are introduced:

$$\frac{\partial \psi}{\partial y} = \rho u$$

$$\frac{\partial \psi}{\partial x} = -\rho v \qquad (2.7)$$

These definitions then result in the following transformations for the derivative":

$$\left(\frac{\partial}{\partial y}\right)_{x} = \rho u \left(\frac{\partial}{\partial \psi}\right)_{x}$$

$$\left(\frac{\partial}{\partial x}\right)_{y} = \left(\frac{\partial}{\partial x}\right) - \rho v \left(\frac{\partial}{\partial \psi}\right)_{x}$$
(2.8)

With these transformations, the conservation equations for momentum, species, and energy then assume the following form:

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u} \frac{dp}{dx} + \frac{\partial}{\partial \psi} \left(\rho u \mu \frac{\partial u}{\partial \psi} \right) \tag{2.9}$$

$$\frac{\partial F_i}{\partial x} = \frac{\partial}{\partial \psi} \left(\frac{L_e}{P_i} \rho u \mu \frac{\partial F_i}{\partial \psi} \right) + \frac{\dot{w}_i}{\rho u}$$
 (2.10)

$$\frac{\partial T}{\partial x} = \frac{1}{c_p} \left\{ \frac{1}{\rho} \frac{\partial p}{\partial x} - \frac{1}{\rho u} \sum_{i=1}^{NS} h_i \dot{w}_i + \frac{\partial}{\partial \psi} \left(\frac{\mu}{Pr} \rho u c_p \frac{\partial T}{\partial \psi} \right) + \rho u \mu \left[\left(\frac{\partial u}{\partial \psi} \right)^2 + \frac{Lc}{Pr} \cdot \frac{\partial T}{\partial \psi} \sum_{i=1}^{NS} c_{p_i} \frac{\partial F_i}{\partial \psi} \right] \right\}$$
(2.11)

O Finite Difference Formulation

For numerical integration the conservation equations are cast into an explicit, variable grid finite-difference form. Using truncated Taylor series expansions around the center point (n, m) in the finite difference shown below,

$$(n, m+1)$$

$$(n, m)$$

$$\Delta x$$

$$\Delta x$$

$$\Delta \psi_{m}$$

$$(n, m-1)$$

the following expressions can be obtained for the derivatives in the lateral direction:

$$\left(\frac{\partial Q}{\partial \psi}\right)_{n,m} = \frac{\Delta \psi_{m} (Q_{n,m+1} - Q_{n,m})}{\Delta \psi_{m+1} (\Delta \psi_{m} + \Delta \psi_{m+1})} - \frac{\Delta \psi_{m+1} (Q_{n,m-1} - Q_{n,m})}{\Delta \psi_{m} (\Delta \psi_{m} + \Delta \psi_{m+1})} (2.12)$$

$$\left(\frac{\partial^{2}\Omega}{\partial\psi^{2}}\right)_{n,m} = \frac{2\left(\Omega_{n,m+1} - \Omega_{n,m}\right)}{\Delta\psi_{m+1}\left(\Delta\psi_{m} + \Delta\psi_{m+1}\right)} + \frac{2\left(\Omega_{n,m-1} - \Omega_{n,m}\right)}{\Delta\psi_{m}\left(\Delta\psi_{m} + \Delta\psi_{m+1}\right)}$$
(2.15)

and, approximately,

$$\left[\frac{\partial}{\partial \psi} \left(e^{\frac{\xi Q}{\delta \psi}} \right) \right]_{n, \, r\alpha} \approx \frac{2a_{n, \, m+\frac{1}{2}} \left(Q_{n, \, m+1} - Q_{n, \, m} \right)}{\Delta \psi_{m+1} \left(\Delta \psi_{m} + \Delta \psi_{m+1} \right)} + \frac{2a_{n, \, m-\frac{1}{2}} \left(Q_{n, \, m-1} - Q_{n, \, m} \right)}{\Delta \psi_{m} \left(\Delta \psi_{m} + \Delta \psi_{m+1} \right)}$$
 (2.14)

where

$$a_{n, m\pm \frac{1}{2}} = \frac{a_{n, m} + a_{n, m\pm 1}}{2}$$
 (2.15)

and, for two-dimensional flow, typically

$$a = \rho u \mu \frac{Le}{Pr}$$
, $\rho u \mu$, or $\rho u \mu \frac{c}{Pr}$

A simple Euler integration is used for integrating in the x-direction; i.e.,

$$Q_{n+1, m} = Q_{n, m} + \left(\frac{\partial Q}{\partial x}\right)_{n, m} \Delta x$$
 (2.16)

Corresponding expressions for the lateral derivatives on the boundary stream-lines can be derived by using the symmetry condition; i.e., setting

$$Q_{n,m+1} = Q_{n,m-1}$$

$$\Delta \psi_{m+1} = \Delta \psi_{m}$$
(2.17)

6 Stability and Axial Step Size

The preceding finite-difference formulation subjects the resulting equitions to a stability criterion governing the maximum allowable step size in the flow direction, Δx . Due to the nonlinearity of the differential equations, the proper stability criterion can only be approximated. For plane flow, the maximum allowable step size at each lateral grid point within the flow field is estimated to be

$$\Delta x \le \frac{\Delta \psi_{m} \Delta \psi_{m+1} (\Delta \psi_{m} + \Delta \psi_{m+1})}{2 (\Delta \psi_{m} a_{n, m+\frac{1}{2}} + \Delta \psi_{m+1} a_{n, m-\frac{1}{2}})}$$
(2.18)

3.0 CHEMICAL REACTIONS

3.1 Rate Equations

Twelve types of chemical reactions are considered as possible contributors to the calculation of the net rate of production, $\dot{w_i}\colon$

Reaction type

Reaction types (7) through (12) correspond to reaction types (1) through (6), but proceed in the forward direction only.

The net rate of production for all reactions is given below in the form $\dot{w}^{(j)} = RP^{(j)} - RM^{(j)}$, which are the symbols used in the computer program.

1.
$$\dot{\mathbf{w}}^{(j)} = \mathbf{k}_f \rho^2 F_A F_B - \frac{\mathbf{k}_f r^2 F_C F_D}{K_p}$$
 (3.2)

2.
$$\dot{\mathbf{w}}^{(j)} = k_f \rho^3 F_A F_B F_M - \frac{k_f \rho^2 F_C F_M}{K_D R T}$$
 (3.3)

3.
$$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C F_D F_E \Omega T}{K_p}$$
 (3.4)

4.
$$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho F_C}{K_p RT}$$
 (3.5)

5.
$$\dot{w}^{(j)} = k_f \rho^2 F_A F_M - \frac{k_f \rho^3 F_C F_D F_M RT}{K_p}$$
 (3.6)

6.
$$\dot{w}^{(j)} = k_f \rho^2 F_A F_M - \frac{k_f \rho^2 F_C F_M}{K_p}$$
 (3.7)

To reduce round-off and truncation errors, $RP^{(j)}$ and $RM^{(j)}$ for each reaction are computed separately. All contributions to the molar rate of production of a given species are then computed and added algebraically to form $\dot{\mathbf{w}}_i$. Since reaction types (7) through (12) proceed in the forward direction only, the second term on the right-hand sides of Eqs. (3.2) through (5.7) is disregarded in calculating the contributions to $\dot{\mathbf{w}}_i$.

In reactions (2), (5) and (6) as well as in (8), (11) and (12), lift denotes a third body species which can be specified. For these reactions the situation often occurs where for various third bodies the respective rate constants differ only by a constant multiplier. These multipliers can be considered as third body efficiencies or weighting factors. If such a case is encountered, the third body species mole mass ratio $\mathbf{F}_{\mathbf{M}}$ becomes effectively a fictitious mole mass ratio, consisting of the weighted sum over all those species having a nonzero weighting factor, i.e.,

$$F_{M} = \sum_{i} f_{i} F_{M_{i}}$$
 (3.8)

where f, are the weighting factors.

3,2 RATE CONSTANTS

The forward rate constant k_f is generally expressed in Arrhenius form. The equilibrium constant, K_p , is determined from the Gibbs free energy difference.

$$\ln K_{p} = -\Delta G/^{c} T \tag{3.9}$$

For speed in computation the rate constants are divided into five types:

Rate Constant Type		
(1)	$k_f = A$	(3.10)
(2)	$k_f = AT^{-N}$	(3.11)
(3)	$k_f = A \exp(B/RT)$	(3.12)
(4)	$k_f = AT^{-N} \exp(B/RT)$	(3.13)
(5)	$k_f = AT^{-N} \exp(B/RT^M)$	(3.14)

4.0 ADAPTATION TO POLLUTION DISPERSION

To solve the CO dispersion cases posed by the TSC, the general model was operated in a mode appropriate to the wind driven stmospheric. Repertion problem. The momentum and energy equations were temporarily to a sed within the computer code since pressure was assumed constant, the velocity profile invariant, and no energy was added or detracted from the expendit system. Additionally, chemical reactions were climinated by assuming frozen conditions for the CO and the remaining atmospheric constituents. This essentially reduces the complex set of conservation equations to one comprised of the species continuity equation, which in the transformed plane is:

$$\frac{\partial F_{i}}{\partial x} = \frac{\partial}{\partial \psi} \left(\frac{L_{e}}{Pr} \rho u \, \mu \frac{\partial F_{i}}{\partial \psi} \right) + \frac{\dot{w}_{i}}{\rho u}$$
 (4.1)

with

$$\frac{\partial u}{\partial x} = 0$$
 and $\frac{\partial T}{\partial x} = 0$ (4.2)

Since chemical reactions were not considered for this analysis, the species production rate \dot{w}_i was utilized to input the pollutant production over the highway width where CO is the i^{th} species. The remaining species are N_2 , O_2 , CO_2 and Ar in proportions corresponding to the standard atmosphere tables. The first term on the right side of the species equation is, of course, the diffusion rate of each species.

Computing the dispersion in finite differences provides a complete description of the pollutant in a vertical plane oriented in a windward coordinate system with x the windward coordinate and y the vertical coordinate. The y coordinate was extended vertically high enough such that the lateral CO gradient approached zero. Integration of the finite difference equations is done in a forward marching sense along the x coordinate; thus information on the dispersion of the CO species is available not only at the receptor site but also at every integration step along the x axis if desired.

O Problem Set-Up

Utilizing the information given, which consisted of the site geometry i.e., number of lanes, width of road, width of center strip, relative location of receptors, and other physical data such as the wind speed and direction, number of automobiles and their speed (average), and the atmospheric stability, the dispersion model was utilized in the following manner.

The problem was initialized at the upwind edge of the road using a vertical wind velocity profile based on the following equation:

$$\overline{u} = \overline{u}_1 (y/y_1)^N \tag{4.3}$$

where \overline{u}_1 is the time averaged wind speed at the measurement point of $y_1 = 18$ ft. The exponent N was based on assuming a roughness height corresponding to short grass, i.e., $N \approx 0.1$ (Ref. 2).

Temperature and pressure were assumed constant throughout the region of the computations as was the distribution of the atmospheric constituents and the background CO concentration.

Calculation of the emission strength was based upon the number of cars, their average speed, and emission factors for CO emission from 1972 EPA data (Ref. 3). A finite area source comprised of the road width and one-limit a car height was used to input the emission data. The source was assumed to be of constant strength across the width of each set of lanes and of zero strength in the median and off the edges of the road.

The wind speed was taken to be uniform in the horizontal plane but varied vertically as mentioned previously. The solution of the CO dispersion equation also requires knowledge of the viscosity coefficient, μ_s which was generated from the following.

$$\mu - \mu_1 (y/y_1)^{M}$$

where μ_1 is the viscosity coefficient at the 2 meter height-from Paggidl (Ref. 2). The exponent M was taken as 0.9 which is related to the roughness reight and atmospheric stability, i.e., M=1-N. The coefficient μ_1 was varied from case to case based on the stability classes provided. A bouyancy effect was included in an approximate manner by displacing upward the emission source using eatitration test cases to fine tune the analysis. This approach was used in line of a rigorous analysis of buoyancy due to lack of sufficient time and atmospheric data from which to derive the appropriate factors.

4.1 INPUT DATA SUMMARY

- 1. Highway geometry
- 2. Emission strength
- 3. Location of emissions in both x and y coordinates
- 4. Wind direction and speed
- 5. Height of mixing layer
- 6. Receptor locations

4.2 OUTPUT SUMMARY

- 1. Continuous vertical (y) distributions of all parameters at desired (prescribed) x (axial) locations.
- 2. Special output at receptor location, both printed and punched cards for CO concentration in PPM.
- CO predictions for both the calibration cases and the remaining site prediction are included as attachments.

5.0 GENERAL COMMENTS

Computation of the emission strength involves several critical assumptions which should be standardized for input to the various models used in future validation projects. Otherwise the comparisons involve not only the various models, but also the assumptions used by each model. Emission factors, for instance, were found to vary widely in the literature depending on the source and when the measurements were made. Perhaps the factors should be specified or at least indicate the source of the data so that each participant uses the same input data. Then only the "model," not one's interpretation of input information is tested.

The height of the stable layer should also be supplied preferably based on measured data at the time the receptor data was taken. This would eliminate an assumption about how high to go with the computations as well as supplying additional information on how the viscosity coefficients should vary with altitude. Definition of the height of the inversion layer would also help in estimating the bouyancy effect.

Some inconsistencies were detected in the calibration case results which were apparently unexplainable in terms of the parameters supplied. One would expect, for instance, that if all other factors were the same for two cases except, say the number of automobiles per unit time, then only the magnitude of the concentration would change. But some cases indicated not only a change in magnitude but also in the gradient (reversed) which would be impossible for any model to predict since the calculational results are always consistent with the input data.

6.0 REFERENCES

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- 2. Pasquill, F., Atmospheric Diffusion, Van Nostrand, New York, 1962.
- Compilation of Air Pollutant Emission Factors, EPA Publication No. AP-42, February 1972.

Attachm | t I | CALIBRATION CASE PREDICTIONS

			R	eceptor Nuri	ber	
Site	Casc					27
No.	No.	1	2	3	4	5
1.1	1	6.4	6.9	5.5		
11	9	3.9	4.0	3.7		
11'	13	7.2	8 • 1	5.7		
11	19	3.5	3.4	3.5		
	. 33	4.3	4.5	4.4		
11	44	4.1	3.9	4.2		
11	47	5.2	5.1	4.5		
11	61	1.5	1.6	1.0		
11	67	4.9	4.3	4+3		
11	80	13.4	13.1	15.7		
11	86	15.1	14.6	13.4		
11	89	4.4	5.1	4.6		
11	93	5.7	6.5	.5+0		
11	98	1.2	1.2	1.3		
11	102	6.5	6.0	5.5		
11	106	3.1	4 - 1	3.4		
11	111	9.0	9.3	8 • 4		
1 1	116	1.9	2.3	2.4		
11	110	4.9	4.6	3.8		
11	141	2.2	1.7	1.2		
11	142	3.1	1.7	1.4		
11	154	6.2	8.4	5.1		
11	165	1.6	1.5	1.7		
11	166	•6	•5	1.8		
	,		• .,			
14	10	1.5	1 • 3	1 • 9	33	
1.4	20	1.4	1.5	1.2		
10	25	4.3	4.3	4.3		
14	27	3.8	2.7	2.7		
1.4	28	3.5	4.0	3.9		
14	35	10.6	9.0	7.7		
14	37	2.2	2.8	2.5		
14	58	1.6	1 • 1	1.5		
1.4	64	4.7	5.2	4.7		
14	68	2.5	2.5	3+1		
14	60	1.9	1.6	2.2		
14	73	5.3	3.8	2.9		
14	83	1 • 4	• 0	• B		
14	94	4.6	4.8	2 • 1		
	0.0		0.4			- 11-
15	23	9•2	9.4	9.9	9.4	95
15	24	8.8	8.4	8.9	8 • 4	8 • 5
15	24	8.2	8.4	8•8	8 • 4	8.5

Attachment II SITE PREDICTIONS

Site	Case	Receptor Number	
No.	No.	1 2	3
11	1	5.0 5.6	4.3
1.1	2	6.8 6.5	5.9
1.1	3	5.8 5.6	5.0
1.1	4	7.0 7.0	6 • 1
1.1	5	5.1 6.1	4+6
1.1	6	4.2 4.3	2.8
1.1	7	4.0 4.3	3.5
1.1	8	2.7 2.5	2.0
1.1	9	3.0 3.4	2.3
1.1	10	6.9 7.2	6.0
1.1	1.1	4+2 5+8	4.7
1 1	12	5.3 6.3	5:3
1 1	13	5.9 7.1	6.5
1.1	14	6.7 7.8	6.5
1.1	15	6+5 6+8	4.9
1.1	16	5 • 6 • 3	5 • 3
11	17	4.8 4.5	4.0
1.1	13	3 • i 3 • 1	2.9
1 1	19	10.6	10.5
1 1	20	4 • 2 5 • 2	4.9
1.1	2.1	6.8 7.3	6+3
1.1	2.2	5.5 6.P	51 - 7
1.1	23	5.0 5.7	5 • 2
1 1	24	5.0 5.1	4.2
1.1	25	4.0 4.3	3.3
1 1	26	3.7 3.8	3.7
1 1	27	4.9 5.2	4.5
1 1	88	5.9 6.7	6 • 1
1 1	29	9.0 9.7	8 • 8
1.1	30	3.9 5.2	4.3
1 1	31	3.9 5.0	4.2
1 1	38	3.1 4.2	4.4
1 1	33	2.0	3 + 3
1 1	34	3.0 4.3	3.3
11	35	5.4 7.3	6+7
11	36	6.9 7.0	6 • 7
11	37	8 4 9 0	8.0
11	38	6.0 6.1	5.3
11	39	5.7 6.5	7 • 1
11	40	13.3 12.4	10.9
11	41	4.2 3.5	5.0
11	42	4 • 4 5 • 4	5 • 3
1 1	43	5.3 7.0	5.9

SITE PREFACTIONS (Continued)

Site	Case	Receptor Number	
No.	ilo.	1 2	
1.1	41	6.4 7.5	6.07
11	45	7.4	4
11	46	6.11 7.1	. 3
1.1	47	4.7	5.3
1.1	413	11 15.7	. 9
1.1	40	4.00	3.9
1.1	50	4.0 3.9	3.7
1 1	51	2.6 3.7	2.7
1.1	52	3.2 3.7	3.0
1.1	53	3.1 4.2	2.6
1.1	54	2.7 3.0	2.7
1.1	6,00	2.10	2.5
1.1	1.7	2.4 2.0	2.7
1.1	57	5.1 4.6	2.45
1.1	GEL	2.7 4.1	2.8
11	59	3.1 3.3	1.9
11	60	2.2 3.5	2.1
1.1	61	3.4 4.2	2.7
1.1	62	3.5 3.9	2.4
1.1	63	4.6	3.1
1.1	64	3+3 3+8	2.9
1.1	65	3 • 1 4 • 1	3.0
1 1	66	4.9 4.4	5.
1.1	67	4.3 3.9	3.3
1.1	68	3.0 4.2	3.5
1.1	69	3 • 1 5 • 4	3.0
11	70	4 • 2 5 • 0	4.6
1.1	71	2.9 4.0	2.8
1.1	72	2.3 2.3	2.0
11	73	5.0 1.9	1 + 7
11	74	3.4	5.2
1 1	75	4.6 4.6	3.9
11	76	4.9 5.5	5.8
11	77	3.9 4.5	3.9
11	78 79	4.1 4.1	4.5
11	80	4.5	4.3
11	81	8.4 8.0	8.3
1 1	82		10.4
11	83		11.7
1.1	84		6.8
1 1	85	7•3 6•9 5•9 7•0	7.0
1 1	86	2.7 3.6	5.7
1 1	87	6.9 7.0	2.3
1.1	BB	6.0 5.6	6.6
11	89		0.3
11	90		3.6
11	91	2.8 4.0 5.0	4.0
1 1	92	1.7 2.1	3.9
11	93	1.2 1.3	1.7
		1 0 1 0 1	1 • 2

SITE PREDICTIONS (Continued)

Site Case	Re	ceptor Nun	ber
No. No.	1	2	3
11 94	1.4	1 • 4	1.3
11 95	2.3	3.2	2.7
11 95	4.0	4.7	4.0
11 97	4.0	4 - 1	0 - 1
11 98	2.3	3.2	3.1
11 99	4.8	4 • B	4.4
11 100	5.8	5.5	5.1
11 101	5.4	6.0	4.5
11 102	3.1	4.5	3.6
11 103	4.2	5.3	4.6
11 104	6.6	8.7	7.2
11 105	7 • 1	8.3	10.2
11 106	5 • 5	7.6	6.8
11 107	2 • 3	3.4	2.6
11 108	2.5	2.6	2.9
11 109	4.2	4.7	4.0
11 110	4 • 1	3.6	3 • 1
11 111	3 • 4	3.1	2.4
11 112	1.2	1.6	1.3
11 113	1 • 3	1.6	1 + 5
11 114	2.6	1.0	1.0
11 115	1+3	2' · O	1 . 7
11 116	1 • 0	°3•1	8:6
11 117	1 • 1	3 - 1	1.6
11 118 11 119	2 • 3	3.4	2.4
11 119 11 120	2.5	3.3	2.6
11 121	2 • 6 2 • 3	3.5 3.3	2.8
11 122	2 • 1	1.3	2.7
11 123	5.0	2.0	2.4
11 124	2.0	2.7	2.1
11 125	2.7	2.4	1.1
11 126	2.5	3.6	1.3
11 127	2.2	3.0	1.6
11 128	2 • 1	3.5	2.0
11 129	1.9	1.9	2.0
11 130	2.1	1.6	1.2
11 131	3.2	3.8	3.0
11 132	2.5	3.9	2 • 1
11 133	2.5	3.5	1.9
11 134	2.7	2.8	2.0
11 135	3.6	2.7	1.9
11 136	3 - 4	2 • 4	3.6
11 137	2 • 1	3.3	1.9
11 138	3.7	3.4	2.6
11 139	10.3	10.2	8.0
11 140	4.6	7.2	6.0
11 141	3.0	3.7	2.3
11 142	5 • 4	7.6	4.7

SITE PREDICTIONS (Continued)

Cit.	C		
	Case	Receptor Number	_
No.	No.	1 2	3
1.1	143	4 • 5 5 • 7	2.1
1 1	144	5+4 6+0	3+5
1.1	145	4 • 4 4 • 1	4 . 1
1.1	146	2.4 4.0	2.5
1.1	147	4.2 5.5	3.6
1.1	148	3.3 4.1	3.6
1.1	149	3.3 4.0	2.6
1.1	150	1.9 2.6	1.6
1.1	151	2.1 2.2	1 * 3
1.1	152	1.7 1.5	1.6
1.1	153	3.0 4.B	3.2
3 1	154	. 3.2 1.4	1 + 7
1.1	155	3 • 1 3 • 1	1 • 2
1.1	156	2 • 4 3 • ?	3.4
1.1	157	2 • 6 3 • 8	2.2
1.1	158	2 • 6 3 • 9	2.5
1.1	159	2.7 2.5	1.6
1.1	160	1.8 1.2	2.5
14	1	3.9 4.5	2.9
14	2	4 • 6 5 • 1	F . 8
14	13	5.3 6.2	4.4
14	4	5.7 6.0	4 - 8
14	67	6+3 5+4	4 - 1
14	6	4.2 4.8	3.6
14	7	3.9 3.6	2.0
14	B	4+8 5+1	3.7
14	9	5.4 5.0	4.2
14	10	4 • 5 3 • 5	3.0
14	1.1	. 3.3 6.6	3.5
14	12	4 • 2 5 • 2	5.0
14	1.3	9 • 5 6 • 5	6 • 1
14	14	5.0 5.8	3.4
14	15	2 • 6 3 • 3	2.4
14	16	2 • 4 2 • 8	2 • 1
14	17	3 • 0 5 • 1	2.6
14	18	3 • 1 5 • 1	3.4
14	19	4 • 3 6 • 1	4.3
14	20	5.9 6.9	4.9
14	21	5.9 7.5	4 • 8
14	22	4 • 0 5 • 1	3.1
14	23	3.8 4.4	3.2
14	24	3.3 3.9	3.1
14	25	2.7 2.5	2.0
14	26	3.1 2.7	2.2
14	27	2.5	1 • 4
14	28	2•1 3•0	2.5
14	29	1.9 · 1.4	1 . 3

SITE PREDICTIONS (Continued)

Site	Case	Receptor Number			
No.	No.		1	2	3
1.4	30		• 6	1.6	5.1
14	31		2.0	2.7	2.0
14	32		3.0	3.0	1.9
14	33		1.9	2.0	2.1
14	34	•	2.9	2 • 5	2 • 1
14	35		2.0	2.5	3 • 4
14	36		1.7	2.8	1 * 8
10	37		2 • 3	3.B	2 • 8
14	38		3 - 1	3.6	2.9
1.4	39		4.3	6.7	4.5
14	40		3.1	2.7	2 . B
14	4.1		4.1	5•0	3.2
14	42		3.7	4 • O	2.6
1 4	4.3		3.3	2.47	2 • 1
14	44		2.6	3.9	2.8
14	45		2.3	4 • 6	1.7
1.4	46		4.6	5 • 4	4+0
14	47		3.6	3.0	2.7
14	48		2.4	3.2	5.9
14	40		2.9	2.5	1.7
14	50		2.7	3 - 1	1.6
14	51		7.5	2.7	2.6
14	52		• 9	1.9	.6
1.4	53		3.9	4 • 4	1 + 8
1.4	54		٦٠1	3 • რ	2.5
10	55		3.3	3.4	2.3
1/4	516		1 + 0	3.5	3+0
14	15-7		3 * (%)	3.0	4.7
14	58		11 . 1	5.3	4.4
14	59		2.9	3 • 1	2.7
14	60		1.9	2.7	2.0
14	61		2.9	2.9	2 • 1
14	62		3+8	3.8	2.6
14	63		3.2	3.3	2.1
14	64		1 • 0	2.7	2 - 1
14	65		2.6	2.5	1.6
14	66		3.6	4.0	1.8
14	67		2.7	3.3	2.6
14	68		3 • 1	2.9	2.9
14	69	•	2.7	2.3	2.2
14	70		6.0	6.7	6.0
14	71		2+8	4 • 1	2.8
14	72		3.9	3.2	2.6
14	73		3.7	7.2	7.2
14	74		1.5	3.8	3.1
14	75		2.7	4 • 1	3.1

SITE PREDICTIONS (Concluded)

Site	Case	Receptor Number					
No.	No.	1	2	3	4	5	
14	76	3.5	4.9	3.7			
14	77	3.4	5.2	4.3			
14	78	3.5	3.2	3.0			
1.4	70	2.6	3.3	3.5			
10	80	3.2	4.0	3.0			
14	81	3 • 4	6.3	3.6			
14	8.8	4 • 1	6.7	6.0			
1.4	83	4 • 1	6.0	4.0			
14	84	4 • 1	4.9	5+0			
14	85	6 • 1	6.9	6.0			
14	86	4.0	5.2	3.5		(4)	
14	87	2.7	2.7	3 • 1			
14	BH	2.4	4 • 4	2.1			
14	69	4.9	3 • 8	3.0			
14	90	6.7	8.7	8.6			
15	1	3 • 5	3.6	3.6	3 • 4	3.6	
1.5	2	4 • O	4.1	5.2	4.4	4.2	
15	3	2 • 4	2.6	2.9	2.5	2.6	
1 45	4	R • 4	8.5	8+5	7.9	8.5	
15	5	6.7	7.0	7.7	6.9	7.2	
1.5	6	10.0	10.1	10.5	10.2	10.1	
15	7	10.0	10.1	10.6	10.2	10.1	
15	8	0.0	0.0	0.5	0.2	0.1	
1 5	9	5 • O	5 • 1	5.8	5.2	5 4 1	
15	10	6 • O	6 • 1	6.7	6.2	6 • 1	
15	1.1	6.0	6.0	6.6	6.2	6.1	
15	1.2	6.5	6.7	7.2	6.7	6.9	
15	13	6 • 4	6.6	7.2	6+6	6 · B	
15	14	7.4	7.6	8.0	7.6	7.7	
15	15	2 • 1	2.1	2.3	2 • 1	2.2	
15	16	2 • 1	2.1	2.3	2.2	2.2	
15	17	3 • 1	3 • 1	3.3	3.1	3.2	
15	18	2.0	2.0	2.6	2 • 1	2.1	
15	19	3.0	3.0	3.6	3 • 1	3.1	
15 15	20	4.0	4.0	4 • 5	4 • 1	4 • 1	
15	21 22	3.0	3.5	4.5	3 • 4	3.7	
15		3.9	4.4	5.3	4.2	4.6	
15	23 24	3.8	4.2	5.0	4 = 1	4.4	
15	25	6.3	6.5	6.8	6.4	6.5	
137	6.73	7 • 3	7.5	7 • 8	7.4	7.5	

C.10 SYSTEMS CONTROL, INC (SCI)

SCI Highway Air Dispersion Models

Overview and Purpose of the Models

The SCI highway air dispersion models predict downwind pollutant concentrations given upwind concentration measurements and the local weather conditions. The basic air dispersion model employed is the Caussian plume dispersion model. The developed model, which is appropriately adapted to account for cut, at-grade, or elevated highways, predicts the downwind concentrations as a function of receptor distance from the highway and receptor height.

Local weather conditions are defined in terms of seven standard stability classes, wind speed, and wind direction. These stability classes define the values of the vertical dispersion parameter, $\sigma_{\rm Z}$, and the horizontal dispersion parameter, $\sigma_{\rm Y}$.

The general equations for the parallel and cross wind components of pollutant dispersion are given as follows (1):

ELEVATED SECTION - ELEVATED RECEPTOR (FOR AT-GRADE, H = 0)

CROSSWIND

$$X = \frac{K_{cc} Q_{c}}{\sigma_{z} \overline{U} \cos \phi} \qquad \left[\exp \left[-\frac{1}{2} \left(\frac{z + H}{\sigma_{z}} \right)^{2} + \exp \left[-\frac{1}{2} \left(\frac{z - H}{\sigma_{z}} \right)^{2} \right] \right]$$

PARALLEL WIND

$$\chi = K_{pe} A \left(\frac{Q_{p}}{U \sin \phi} \right) \left(\frac{30.5}{w} \right) \left[\exp \left(-\frac{1}{2} \left(\frac{y}{\sigma_{y}} \right)^{2} \right] \right]$$

$$\bullet \left[\exp \left(-\frac{1}{2} \left(\frac{z + H}{\sigma_{z}} \right)^{2} + \exp \left(-\frac{1}{2} \left(\frac{z - H}{\sigma_{z}} \right)^{2} \right) \right]$$

CUT SECTION - ELEVATED RECEPTOR

CROSSWIND

$$\chi = \frac{K_{cc} Q_c}{\sigma_z \overline{U} \cos \phi} \quad \left[\exp + \frac{1}{2} \cdot (\frac{z}{\sigma_z})^2 \right] \quad \left[\exp - \frac{1}{2} \cdot (\frac{z}{\sigma_z})^2 \right]$$

PARALLEL WIND

$$\chi = K_{pc} A \left(\frac{Q_p}{U \sin \phi} \right) \left(\frac{30.5}{w} \right) \left[\exp \left(-\frac{1}{2} \left(\frac{y}{\sigma} \right)^2 \right) \left[\exp \left(+\frac{1}{2} \left(\frac{z}{z} \right)^2 \right) \right]$$

$$\bullet \left[\exp \left(-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right) \right]$$

where

 $\chi = Concentration of pollutant 3m/m³$

Q = Crosswind emission source gm/sec -m

 $Q_{\rm D}$ = Parallel wind emission source gm/sec

U = Wind speed m/sec

 ϕ = Angle of wind where 0° is perpendicular to highway

y = Straight line distance from highway edge

z ' = Height of receptor above level ground

H = Effective height of highway above surrounding terrain

z = Vertical dispersion coefficient

ທູ = Norizontal dispersion coefficient

w = Width of roadway m

= Depth of highway cut m

A = Downwind concentration ratio for parallel winds

 K_{ce} , K_{pe} Empirical coefficients that relate to characteristics of the roadway being modeled. Determined by field measurements.

The methodology used to determine downwind concentration predictions with these equations is described in section II. An analytical . Togy that can be used to assess the sensitivity of the predictions to unconstant. In the model and weather parameters is discussed in section III. Specific a plication of the models to the three TSC cases 11, 14, and 15 is presented in section IV.

II. Prediction Methodology

Pollutant concentration on the upwind side of the highway consists of two parts, a constant ambient component and a spatially varying, parallel wind component. On the downwind side of the highway, the pollutant concentration can be divided into three parts, two of which are the ambient and parallel components, and the third which is the crosswind component.

The calibration of the dispersion models for a given highway with available field data is performed with the following steps:

- 1) Fach data sample (where a sample is defined as the set of upwind and downwind data points measured at the same time instant) is considered. For example, one may have 25 data samples, each of which has 5 upwind measurements and 3 downwind measurements. For each, use the upwind data to estimate the ambient and parallel wind components. This estimation is performed by regression fit of the data to the parallel wind dispersion model and the assumed constant ambient component.
- 2) The calculated parallel component model is used to estimate the parallel wind component concentration at the locations of the downwind measurements.
- 3) The estimated parallel wind component concentrations and the estimated ambient concentration are subtracted from the measured downwind concentrations.

4) The resulting downwind residuals from all data samples are used to calibrate the crosswind air dispersion model. Calibration is performed by regression fit of the data to the rodel.

After calibration of the models, downwind concentrations are predicted from given upwind concentrations in the following way:

- For each upwind concentration data sample, the ambient and parallel wind contributions are determined by regression methods.
- 2) The downwind receptor concentration values from the parallel wind component are calculated from the resulting parallel wind component model.
- 3) The downwind receptor concentration values from the crosswind component are calculated from the calibrated crosswind model.
- 4) The total downwind receptor concentration values are the sum of the ambient, the parallel wind, and the crosswind concentrations.

The calibrated parallel and crosswind models can be used, for specified ambient concentration levels, to predict up-and-down wind concentration levels at that road site. This prediction capability would be employed in environmental impact analysis.

III. Parameter Sensitivity Assessment

The predictions from the above described air dispersion models are subject to two types of uncertainties -- uncertainties in the value of the

modeling parameters (e.g., wind speed, σ_z , σ_y) and uncertainties in the correct structure of the model. Uncertainties in the structure of the model can only be analyzed by comparing the model results with the results of other model: (e.g., box model). On the other hand, the impact of uncertainties in the modeling parameters on the model predictions can be expressed analytically.

Given the function,

$$x = F(x_1, x_2, x_3, \dots, x_N)$$

where \mathbf{X}_1 might be wind speed, \mathbf{X}_2 might be source strength, one can, assuming that the variables \mathbf{X}_1 are statistically independent and gaussian, express the variance of χ as,

$$\operatorname{Var} \chi = \sum_{i=1}^{N} \left(\frac{\partial \overline{F}}{\partial X_{i}} \right)^{2} \quad \operatorname{Var} X_{i}$$

where $\frac{\partial \overline{F}}{\partial X_{\underline{i}}} \stackrel{\Delta}{=} \frac{\Delta}{}$ the partial derivative of F with respect to $X_{\underline{i}}$ evaluated at the expected (mean) values of the $X_{\underline{i}}$.

From this formula, the variance of χ can be expressed in terms of the contribution of uncertainty from each parameter X_1 .

SCI has coded this variance relationship for the gaussian plume model. Estimates of the uncertainties of the model parameters can thus be used to directly determine the variance of χ .

IV. Processing of TSC Test Cases

Data was received from TSC for 3 roadway sites = 11, 14, and 15. Each of the three data sets contained calibration data (upwind and corresponding downwind measurements) and nodel validation data (upwind measurements from which downwind predictions were to be made).

Because of the wide center strip, the concentrations upwind and downwind for site 11 are assumed to be the superposition of two line sources representing the two sets of highway lanes. The three upwind ressurements of a data sample are used to compute the coefficients associated with the ambient and parallel wind concentration components (winds with direction -12" to 12" or 168° to 192° are considered to have only a crosswind component, winds with direction 75° to 102° or 258° to 282° are considered to have only a parallel wind component, winds in other directions are considered to have both parallel and crosswind components). From these coefficients the downwind concentration predictions for the model validation data are computed with the methodology described in section II. Values are computed for $\boldsymbol{Q}_{_{\boldsymbol{Q}}}$ and $\boldsymbol{Q}_{_{\boldsymbol{p}}}$ with equations specified by reference (1). These values are a function of average vehicle speed and emission factor (that accounts for model year, emission standards, ctc.). The value of W is 36' for each section of the divided road. Values of A are taken from reference (1). Predictions were made on all model validation data.

Site 14 data was processed in principle like the site 11 data since three downwind measurements were available for each data sample. The only major difference was that the highway was considered as a single emission line source, because of the narrow median strip, as opposed to the double line source used for site 11. The methodology described in section 2.0 was applied with the parallel and crosswind models identified in section 1.0.

Site 15 is a highway elevated 25 feet above the parrounding terrain. Site 15 presented difficulties to the modeling approach described in meetion 2.0 because the number of upwind measurements per sample point is one who leas the minimum number of points required is three. Consequently, the approach was slightly modified in order to utilize the available data.

In order to obtain more than two upwind data points per "data sample" for both the calibration and model validation data, these data sets were organized into subgroups according to the measured meteorological conditions. The three calibration data samples (#23, 24, and 25) were grouped together to estimate the calibration parallel, cross and ambient wind components. The validation data were divided into the following subgroups in order to perform downwind concentration estimates:

Subgroup	Pata Sample Points in Subgroup.
1	4, 5, 12, 13, 14
2	1, 2, 18, 19, 20
3	3, 21, 22, 23
4	9, 10, 11
5	15, 16, 17

Data sample points 6, 7, 8, 24, and 25 were not processed because they could not be satisfactorily placed into a subgroup with 3 or more data sample points.

The effective roadway height was selected to be 29 feet, the additional four feet being the result of air turbulence resulting from the traffic flow (as suggested by reference 1).

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C.11 SYSTEMS, SCIENCE AND SOFTWARE (SSS)

EXPLOR

EXPLOR is an acronym standing for Examination of Pollution Levels Of Roadways. The EXPLOR finite difference, advectional diffusion computer code has been developed by Systems, Science and Software to predict the impact of a highway on local air quality from the roadway edge to 1000 feet from the roadway. EXPLOR requires meteorological data, consisting of wind velocity and stability class identification, and traffic information, consisting of traffic counts, and pollutant emission factors. Explor is designed to handle cut, fill, and at-grade roadway geometries, viaducts, and split freeways at the same or different levels.

The mathematical basis of EXPIOR is the numerical, finite-difference solution of the advection-diffusion equation describing the conservation of mass of the pollutant, i.e.,

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \vec{\nabla} c = \vec{\nabla} \cdot (\underline{k} \cdot \vec{\nabla} c) + s \tag{1}$$

where

c = pollutant concentration

u = mean wind velocity

k = turbulent diffusivity tensor

S = emission source strength

In this framework, the pollutant is advected by the mean fluid motion and dispersed by the turbulent mixing processes, as modeled by the diffusivity terms, $\vec{\nabla} \cdot (\mathbf{k} \cdot \vec{\nabla} \mathbf{c})$, in Equation 1. The emission of pollutants is modeled by the inclusion of the source term,

S. Basically, pollutants are introduced at source cells, and at each time step, At, a metered amount of pollutant is added to the source. The pollutant is advected and diffused by the winds until steady state is reached.

Both advection and diffusion are treated in the code by using a Crowley second-order scheme. In EXPLOR, any quantity, Ω_r to be advected in the x-direction (for example) is given by

$$\Omega^{n+1} = \Omega_{i}^{n} + \frac{\Delta t}{\Delta x_{i}} (F_{i} - F_{i+1})$$
 (2)

where Δt is the time step, the i subscript denotes the zone manber, and F is a flux term which is a function of the form

$$F_{i} = [(u\Omega)_{(i+1)} - (u\Omega)_{i}], \qquad (3)$$

u being the x-velocity component. Diffusion is treated by replacing the mean velocity in Equation 3 with a diffusion transport velocity.

It is evident that wind-field $(\dot{u}(x,y))$, diffusivity formulation $(k(\dot{u},x,y))$, and source models (S) are required to numerically integrate Equation 1. The wind-field calculation should include both tangential and vertical components of the velocity. Since reads are located in the near surface atmospheric boundary layer, the vertical gradient of the tangential velocity must be taken into account, as well as the variations in eddy diffusivity in the rear surface region. These effects have been incorporated into the EXPLOR model.

The wind field in EXPLOR calculations is computed by taking into account the wind shear that exists in the near surface atmospheric boundary layer. The usual definition of the velocity potential, i.e.,

$$\vec{u} = \vec{\nabla} \phi \tag{4}$$

is modified by a potential coefficient tensor, λ ,

$$\vec{\mathbf{u}} = \underline{\lambda} \vec{\nabla} \phi \tag{5}$$

when $\underline{\lambda}$ can be prescribed to fit the wind conditions to be simulated. In EXPLOR, the current prescription for λ_{ij} is

$$\lambda_{ij} = 0, i \neq j \tag{6}$$

$$\lambda_{11} = (z/z_0)^p \tag{7}$$

$$\lambda_{22} = \lambda_{33} = 1$$
 (except at boundaries where (3) $\lambda_{22} = 0$)

where

z = height above the ground

zo = reference height

p = coefficient which is a function of stability class

Note that with this prescription of $\underline{\lambda}$ (Equations 6 and 7), the linear field, $\phi \propto x$, will automatically reduce to a sheared profile consistent with the specified stability class.

In general, the prediction of the turbulent diffusivity at an arbitrary point in the wind field is based on the relationship that

where

k = diffusivity

u' = turbulent fluctuation velocity at which turbulent energy is maximized

£ = turbulence length scale

The EXPLOR model incorporates a model where

$$k_{22} = 0.45 \, \operatorname{u\sigma}_{\varepsilon} \ell \tag{10}$$

where

u = local wind speed

 σ_{ϵ} = mean wind vane fluctuation

Both σ_ϵ and ℓ are functions of the Pasquill stability class and height above the ground.

The wind field is calculated by solving the continuity equation, i.e.,

$$\vec{\nabla} \cdot \vec{\mathbf{u}} = \mathbf{0} = \vec{\nabla} \cdot \underline{\lambda} \vec{\nabla} \phi \tag{3.1}$$

in a finite difference grid which includes block models of major topographical features and structures that present important slip boundaries to the flow.

In practice, ϕ , is obtained by assuming an initial value and then using the line successive over-relaxation technique, where

$$\phi_{ij}^{n+1} = \alpha \phi_{ij}^{n+1} + (1-\alpha) \phi_{ij}^{n}$$
(12)

where

 $\alpha > 1$

n = iteration number

Experience has shown that the solution converges ($\phi^{n+1} \approx \phi^n$) after twenty iterations.

The horizontal wind (which is boundary centered) is calculated from

$$u = \sum_{ij} \cdot \frac{(\phi_{ij} - \phi_{i-1,j})}{\Delta x_{i-1}^{a}}$$
 (13)

where Δx is the distance in the x-direction from cell center to cell center and ϕ is cell centered.

The horizontal wind field is then modified by the input data to provide a least-squares fit between the calculated wind field $(\mathbf{u}^{\mathbf{C}})$ and the given wind data $(\mathbf{u}^{\mathbf{m}})$ by taking

$$\delta = \frac{\sum_{i=1}^{n} u_{i}^{c} u_{i}^{m}}{\sum_{i=1}^{n} u_{i}^{c} u_{i}^{c}}$$
(14)

when n = number of wind data sets input.

When

$$u = u^{C} \delta \tag{15}$$

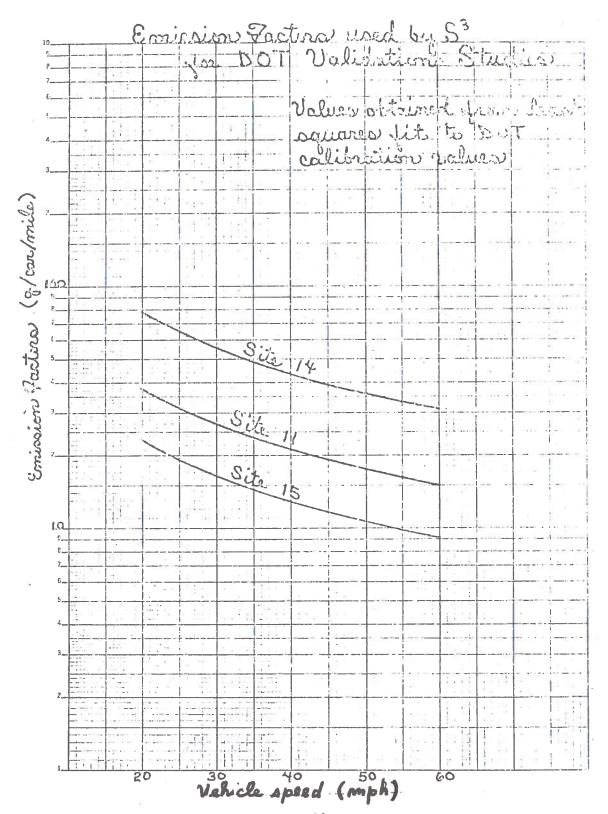
where u= final wind value. Note that for only one wind measurement, next, $u=u^m$.

The vertical wind is obtained by solving

$$\vec{\nabla} \cdot \vec{u} = 0 \tag{16}$$

in the finite form

$$v_{ij} = v_{i,j-1} + \Delta y_j \frac{(u_{i,j} - u_{i+1,j})}{\Delta x_i}$$
 (17)



C.12 TSC/EPA

TSC/EPA Highway Line Source Model

John Zimmerman, EPA David S. Prerau, TSC Paul J. Downey, TSC

INTRODUCTION

The TSC/EPA Highway Line Source Model is an air pollution dispersion model of the Gaussian class. The computer program for this model was originally written by John Zimmerman, EPA National Environmental Research Center, Research Triangle Park, North Carolina. Major modifications to the original model were subsequently made by Dr. David S. Prerau and Paul J. Downey of the U. S. Department of Transportation/Transportation Systems Center, Cambridge, Massachusetts. The model program is written in FORTRAN IV. Examples of its usage for modeling a highway, a street, or a complex multilevel interchange are discussed in References 1 and 2. DESCRIPT: ON

The Model can calculate the pollutant concentrations at any number of receptors produced by any number of straight line segment sources of uniform emission. A complex set of roadways, e.g. an interchange, can be modeled by a large set of line segment sources. The Model can handle upgrade and downgrade roads as well as horizontal roads.

The Model first calculates the location of line sources to represent each lane of each road segment, based on the location of the center line of the road, the road width, and the width of the center strip. Then it calculates the concentration at each receptor due to each line source. Finally,

it sums the contributions at each receptor due to each land of each road segment to produce the final computed concentration.

The concentration due to a single line source at a receptor is given by:

$$C(R) = \int_{0}^{L} Q_{s} P_{R}(\ell) d\ell$$

Where:

C(R) is the concentration at receptor R

L is the length of the line source

Q is the line source strength

 $P_R(\ell)$ is the concentration produced at R by a unit strength point source located a distance—from the end of the line source.

To compute the integral, the Model divides the line source into smaller line source segments and computes the sum of the contributions of each segment to the pollutant concentration at the receptor. The line source is divided into progressively greater numbers of smaller line source segments until successive calculated values of pollutant concentration seem to have converged. The contribution from each small line source segment is calculated by the trapezoidal rule, which approximates the contribution to the integral by a small line source segment as the average of the contributions of point sources located at each end of the segment. Thus, the above equation becomes:

$$C(R) = \frac{Q_{s}}{N} \left[\frac{P_{R}(0) + P_{R}(\frac{L}{N})}{2} + \frac{P_{R}(\frac{2L}{N}) + P_{R}(\frac{L}{N})}{2} + \cdots \right] + E_{N}$$

$$= \frac{Q_{s}}{N} \left[\frac{1}{2} P_{R}(0) + \sum_{i=1}^{N-1} P_{R}(\frac{iL}{N}) + \frac{1}{2} P_{R}(L) \right] + E_{N}$$

Where:

N is the number of line source segments of $\frac{L}{N}$ into which the line source has been divided.

 $\boldsymbol{E}_{\boldsymbol{N}}$ is the error term (which decreases as N increases).

Thus, each step in the calculation of the concentration due to the line source is reduced to the calculation of the concentrations at the receptor due to N point sources. N is continually doubled until a convergence criterion is met.

To calculate the concentration at a receptor due to a point source, the TSC/EPA Model uses the following equation adapted from Reference 3:

$$P_{R}(x,y,z,H) = \frac{1}{2\pi U \sigma_{y} \sigma_{z}}$$

$$\exp\left(\frac{-y^{2}}{2\sigma_{y}^{2}}\right) \left[\exp\left(\frac{-(z-H)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(\frac{-(z+H)^{2}}{2\sigma_{z}^{2}}\right) + \sum_{N=1}^{J} \Lambda(N)\right]$$

$$A(N) \triangleq \exp\left(\frac{-(z-H-2NL)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(\frac{-(z+H-2NL)^{2}}{2\sigma_{z}^{2}}\right)$$

$$+ \exp\left(\frac{-(z-H+2NL)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(\frac{-(z+H+2NL)^{2}}{2\sigma_{z}^{2}}\right)$$

Where:

- P_R is the concentration point at receptor R which is located at point (x,y,z) due to a unit point source of pollution located at point (0, 0, H). [x is the downwind distance; y is the crosswind distance, z is the vertical distance].
- U is the wind speed
- σ_y a function of x, is the standard deviation of concentration in the crosswind direction.
- $\sigma_{\rm Z}$ a function of x, is the standard deviation of concentration in the vertical direction.
- L is the height of the mixing layer.
- J is chosen such that N=J is the first value of N such that A(N) is less than a given small constant.

This equation is a form of the standard Gaussian plume model of air pollution dispersion. The first exponential accounts for crosswind dispersion. The first z exponential gives the contribution of pollution directly
from the source. The second z exponential gives the contribution of pollution which was reflected from the ground. The A(N) terms account for
multiple eddy reflections from both the ground and the stable layer.

The TSC/EPA Model considers multiple wind directions, rather than a single wind direction, and computes principal wind direction concentrations by sector averaging. It is possible for the worst-case traffic and meteorological conditions to occur for any wind direction. Since the wind direction is a variable of primary importance in the determination of t'e pollutant concentration produced at a given receptor by a given road configuration, it is desirable to consider many wind directions for each situation considered. Therefore, the Model iterates on wind direction so that results for several wind directions can be produced sequentially

in one Model run. From these results, the worst-case wind direction can be chosen for each receptor, and thus the worst-case results can be used. In general the worst-case wind direction will be different for each receptor.

Due to the well known variability of wind direction at the low wind speeds usually considered in worst-case computations, a sector-averaged pollutant computation of the following form is used:

$$C_{SA} = \frac{1}{4} \left[C(\theta_n - 22.5^\circ) + 2C(\theta_n) + C(\theta_n + 22.5^\circ) \right]$$

Where

 c_{SA} is the sector-average pollutant concentration for a principal wind direction.

C(0) is the calculated concentration for wind direction

 θ_{n} is the nominal angle for the principal wind direction. Using the multiple wind direction capability, sixteen different runs are made using wind directions every 22.5°. The Model then automatically computes the pollutant concentration at each receptor for each principal wind direction, using sector averaging.

INPUTS

- 1. The endpoints of the center line of each road segment.
- 2. The width of each road segment.
- 3. The width of the center strip of each road segment, if any.
- 4. The height of emissions for each road segment.
- 5. The emission strength of each lane of each road segment.

- 6. The wind directions to be used.
- 7. The wind speed.
- 8. The height of the mixing layer.
- 9. The coordinates of the receptors.
- 10. The ground heights (if non-zero) at each road segment endurant and at each receptor.

OUTPUTS

- 1. The endpoints of the center line of each road segment.
- 2. The width of each road segment.
- 3. The width of the center strip of each raod segment, if any.
- 4. The height of emissions for each road segment.
- 5. The emission strength of each lane of each road segment.
- 6. The wind directions to be used.
- 7. The wind speed.
- 8. The height of the mixing layer.
- 9. The coordinates of the receptors.
- 10. The ground heights (if non-zero) at each road segment endpoint and at each receptor.
- The predicted concentration at each receptor for each wind direction considered.

REFERENCES

- Eugene M. Darling Jr., David S. Prerau, and Paul J. Downey, Computer ANALYSIS OF AIR POLLUTION FROM HIGHWAYS, STREETS AND COMPLEX 100 OCCUMAGE., A CASE STUDY: PORTIONS OF THE PROPOSED 3-A SYSTEM IN 1978 BANTHOOR, MARYLAND, Report No. DOT-TSC-OST-73-37, U. S. Department of Tran Dortetion/Transportation Systems Center, Cambridge, Massachusetts, March 1971.
- Eugene M. Darling Jr., David S. Prerau, Paul J. Bowney, and Jeffrey D. Garlitz, AN AIR QUALITY ANALYSIS OF A "MULTILEVEL CONTIEX INTEGRATED AN APPLICATION OF THE UPGRADED TSC/EPA MODEL, U. S. Department of Transportation/Transportation Systems Center, to be published in 1975.
- D. Bruce Turner, WORKBOOK OF ATMOSPHERIC DISPERSION ESTIMATES, Public Health Publication No. 999-AP-26, U. S. Environmental Protection Agency, 1970.

WALDEN HIGHWAY MODEL

INTRODUCTION

The Walden Highway Model is an air pollution diffusion model based on the Gaussian Plume equation. The computer program for the Walder. Highway Model is a modified version of the Air Quality Display Model (A.P.M) [1], criginally developed under EPA sponsorship and adapted for computer applications by Martin and likvard [2]. This multiple-source model has received extensive application by Federal and State regulatory equations in evaluating regional air pollution control strategies. The adaptation of this computer model to the current highway application for careon monoxide (CO) concentrations was made by Walden Research Division of Abcor, Inc., Cambridge, Massachusetts.

Two major modifications were made to the AQDM program. First, a program module VEHEMI was integrated into the Fortran IV source code to accurately determine vehicle emission rates for CO. VEHEMI is designed to compute explicitly the CO emission rate (grams/vehicle mile) for a specified motor vehicle model year mix. In this case, the mix is typical of an urban area on the East Coast in 1972. The method is based on a procedure by Kircher and Armstrong [3] and incorporates such considerations as deterioration and speed adjustment factors. Recent changes in federal automotive emission standards related to amendments to the Clean Air Act of 1970 have been incorporated. Secondly, a unique method for transforming highway line sources into series of point sources was incorprorated into the model to conform to the input-output formats desired in the current application.

DESCRIPTION

The basic univariate Gaussian diffusion equation for the concentration at an elevated receptor due to an elevated point source is given by the expression:

$$\chi(x, y, z) = \frac{0 (c-y/c)}{\sqrt{2\pi} \sigma_z u} \left(\frac{2\pi x}{16}\right) \left\{ \exp\left(-\frac{1}{2}\left(\frac{Z-H}{\sigma_z}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{Z-H}{\sigma_z}\right)^2\right) \right\}$$

 $X(x, y, z) = pollutant concentration at receptor point (x,y,z),(gns/n^3).$

Q = emmission rate, (gms/sec). u = mean wind speed, (m/sec).

 σ_z = standard deliation of the plume concentration distribution in the vertical direction, (m).

H = height of the point source, (m). (x,y,z) = coordinates of the receptor relative to the point source, (a).

c = width, at the receptor, of a 22.5-degree circular sector centered on the point source.

The Gaussian equation is based upon several assumptions, including:

- (a) Total reflection of the plume takes place at the earth's survivo.
- (b) The plume description represents conditions averaged over a time period of several minutes. The "instantaneous" behavior of the plume, particularly during unstable atmospheric conditions is more complex.
- (c) The effluent has neutral buoyancy in the atmosphere: no fall-out or buoyancy rise is modeled by the equation.
- (d) The time-averaged plume exhibits a Gaussian distribution of concentration, in the vertical dimension. The measure of the spread in this direction (the dispersion coefficient) is considered to be a function of downwind distance and atmospheric stability only.
- (e) The plume is a steady-state phenomenon resulting from a constant, continuous emission source, and none of the effluent "disappears" (by chemical change or by absorption of the ground surface, for example). Thus, an area integration of the plume conentration in any plane perpendicular to the center line is constant, regardless of the downwind distance.
- (f) Pollutant dispersion in the crosswind direction is modeled using linear interpolation within a 22.5-degree circular sector, corresponding to the 16-point compass used in wind direction measurements.

All diffusion calculations made by the Walden Highway Model use this Gaussian equation. The model treats a highway line source by first breaking it up, one lane at a time, into an aggregate of many small area sources, each about 40 square meters in size, arranged in a line. Each area source is then converted to a "virtual" point source located upwind of the center of the area. The "virtual" point is placed at such a distance upwind that the 22.5-degree sector used in the calculations subtends the area width.

The values of σ_Z used in this model are Turner's "Workbook" dispersion coefficients [4] plus 1.7 meters. The "Workbook" coefficients are widely used and are based on field trial data representative of diffusion at or near the ground. The additional 1.7 meter spread is to account for an initial vertical distribution of the emissions, as they diffuse from the roadway edge, due to mechanical turbulence caused by traffic flow. Note that the Gaussian distribution used in the vertical dimension accounts for the elevation of toth the highway emissions source and the receptor probe, and the reflection of the plume at the earth's surface.

The CO concentration as calculated is modified by two scaling factors before being output. First, it is multiplied by 0.7374, a factor to convert the averaging time of the concentration from the 10 minutes characteristic of σ_z , to the desired 1-hour period [4]. This time scaling factor will give a conservative estimate of the 1-hour concentration. Finally, a factor of 817. is used to correct the units from grams per cubic meter to parts per million of CO.

REFERENCES

- Air Quality Display Model, prepared for National Air Pollution Control Administration under contract No. PH 22-68-60, November 1969.
- Martin, D. O. and Tikvart, J. A., "A General Atmospheric Model for Estimating the Effects on Air Quality of One or More Sources", presenced at 61st Annual Meeting, APCA, St. Paul, Minnesota, June 1968.
- 3. Kircher, D. S. and Armstrong, D. P., An Interim Report on Motor Vehicle Emission Estimation (Draft), EPA Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina, October 1972.
- 4. Turner, D. B., Workbook of Atmospheric Dispersion Estimates, PHS Publication No. 999-AP-26, (Revised), 1969.

APPENDIX

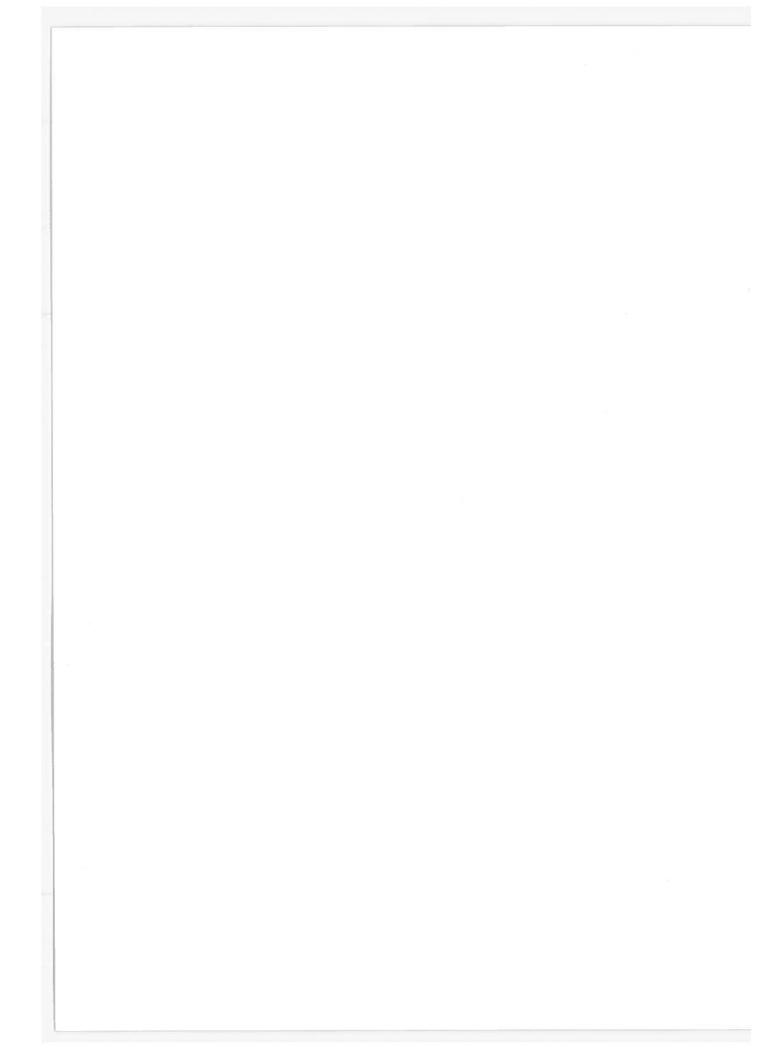
Input

- The site number.
- 1. 2. 3. 4. The case number.
 The total vehicles per hour on the highway segment.
 The average traffic speed.
 The stability class.
 The wind direction.

- 6.
- The wind speed.
 The background concentration at three upwind receptors.

Output

- 1. 2. 3. The site number.
- The case number.
- The predicted concentration at five downwind receptors.



APPENDIX D. COMMENTS OF COMPANIES ON VARIOUS

ASPECTS OF THIS STUDY

AEROVIRONMENT INC.

660 SOUTH ARROYO PARKWAY PASADENA, CALIFORNIA 91105

(213) 449 4392

June 18, 1974

Mr. Robert E. Valente
Department of Transportation
Transportation Systems Center
Kendall Square
Cambridge, Massachusetts 02142

Dear Mr. Valente:

Enclosed is a brief description of our model which you requested to accompany the results of our AVQUAL model test runs using data provided by TSC. Those test runs were submitted at an earlier date.

Also enclosed is our billing for work performed on this project in accordance with TSC's letter contract dated February 7, 1974.

We would like to know the results of these evaluations if appropriate.

Sincerely yours,

SBabo 22

Lal Baboolal Research Scientist

LB:lp Enclosures The Center for the ENVIRONMENT & MAN, Inc. 275 Windsor Street • Hartford, Connecticut 06120 293 545/4400



June 20, 1974

Mr. Paul Downey U.S. Dept. of Transportation Transportation Systems Center Kendall Square Cambridge, Mass. 02142

Subject: P.O. #TS-8138

Dear Mr. Downey:

Enclosed with this letter is a statement concerning the running of the CEM Highway Traffic-Air Pollution Model with the data you supplied. Also enclosed is a deck of cards required by subject order.

We at CEM regret the delay in submitting this data and hope that you were not unduly inconvenienced. After review of the enclosed information, should you have any questions of a technical nature Mr. G. Anderson may be contacted at (203) 549-4400, ext. 390. Questions of a business or financial nature may be directed to the undersigned at (203) 549-4400, ext. 398. We at CEM appreclate the opportunity to participate on this study. We hope review of the models will lead to the conclusion that future work with CEM in this area would be useful to your organization.

Very truly yours,

THE CENTER FOR THE ENVIRONMENT & MAN, INC.

R.J. Dolan, Jr

Director, Business Administration

/kls Enc.

cc: R.E. Chandler (DOT)

ENVIRONMENTAL RESEATED A REPORT OF THE MENTINGER OF THE PROPERTY OF THE PROPER

REF: 074-005-MR-516

ERT Project No.: P-1090

29 May 1974

Mr. Paul J. Downey Transportation System Center 55 Broadway Cambridge, Massachusetts 02142

Dear Mr. Downey:

We are enclosing the IBM punched-card outputs of our dispersion model calculations which we have undertaken in accordance with your purchase order TS-8154. We have performed the calculations corresponding to all of the calibration and validation cases supplied to us within the allotted bedget. In addition we enclose a brief description of the dispersion model used in this program.

Having recognized that some of the calibration run data set was collected by ERT for the District of Columbia Department of Highways and Traffic (DCDMT), we feel that certain points should be brought to your attention in order to assist you in interpreting the results of your study. In checking the input data supplied for the model evaluation runs, we noted some errors in the site (cometry and in the units used to express certain meteorological parameters. We feel that in fairness to other participants in your evaluation program, you should be made aware of the following discrepancies:

- The actual width of the center strip at the Independence Avenue nonitoring site (Site 11) was about 12 feet - not 95 feet.
 This should lead to substantial underpredictions of concentrations at the indicated downwind distances by participants who were unaware of this fact.
- 2. The three calibration cases for Site 15 (Anacostia Freeway), supplied wind speeds of 7 meters/second. In reviewing our cwn data, we note that during the actual monitoring situations, the winds were recorded as 7 mph. Most models calibrated to correspond with the former wind speeds could be expected to underpredict highway contributions to CO concentrations at this site by about a factor of two.

REF: 074-005-MR-516

3. We noted that a large number of calibration cases used measurements obtained during times of very low traffic volumes. In our analysis of the overall data set, we concluded that the best cases for model validation purposes were those with relatively large volumes. The problem appears to be that in an urban setting, the times of day corresponding to low traffic volumes are characterized by large background contributions. Thus, the roadway contributions to measured concentrations at the sites are small compared to background levels under those circumstances. For this reason, mode, predictions of the highway-induced downwind concentrations are generally lower than those observed, since the local traffic impact on air quality is essentially in the 'noise level' of the background values when traffic volumes are very light. In our validation program for the DCDHT, we did not use such cases for the evaluation of our model.

Finally, we would like to provide you with a few comments regarding the calculations we have done for your study:

- We have performed the calculations for your study without any attempt to calibrate our model with the calibration data supplied. We did, however, run the model for all calibration cases, using correct input parameters where discrepancies were found to exist.
- For the Site 11 runs we used the correct (12-ft) median strip width as an input value. This was done in agreement with the understanding of a phone conversation between yourself and John Lague of ERT.
- 3. Emission rates were calculated using the ERT program VEMIT which converts traffic volume, speed, and yearly mix distribution into 'line source' emission rates in units of gm m⁻¹ sec⁻¹. A 1972 Eastern U. S. traffic mix was assumed for these computations, with a 5% heavy duty vehicle makeup.
- 4. The calculated concentrations for Site 15, Case 8 reflect only highway contributions, since no background value was supplied for this case.

REF: 074-005-MR-516

If you have any questions concerning this work, or if we can be of any further assistance, please feel free to call either myself or John Lague.

Sincerely,

Bruce A. Egan, Sc.D. Technical Director

Environmental Sciences Division

BAE/jc

Enclosure



ENVIRONMENTAL CONSULTANTS LTD.

603 - 7TH AVENUE S.W., CALGARY, ALBERTA, CANADA T2P 2TH PHONE (403) 264-5112 2000 WEST LOOP SOUTH, HOUSTON, TEXAS 77027, U.S.A.

PHONE (713) 611-6393

May 31, 1974

U. S. Department of Transportation Transportation Systems Center Kendall Square Cambridge, Massachusetts 02142

Attention: Mr. Paul Downey

Reference: TCD

Dear Mr. Downey:

Attached you will find a summary of our results for the model validation experiments conducted by TSC. The output is in the form of punched cards as requested. A summary of the technical approach and model description is also enclosed.

In the technical approach section, I have attempted to outline the limitations in describing the site, roadway length, etc., which necessitated making assumptions before the cases could be calculated. As an example, without a calibration phase or TSC specifying the emission levels and distribution vertically per lane, there could be quite a range in answers due to this uncertainty alone.

Perhaps other companies have had considerably more experience in traffic modeling and could determine from the provided data what emissions to use. Our experience in traffic modeling is limited and thus the emission distribution factors alone introduced considerable uncertainty. In future validation exercises, we would find it preferable for TSC to define the emission characteristics and then the diffusion characteristics could delineate the best modeling approach.

If you have questions regarding the enclosed model description or the results, please contact me.

Sincerely,

Executive Vice President

RBL:jc Enclosures

KARSAN SCIENCES CORPORATION A KAMAN COMPANY

1500 Garden of the Gods Kond Mailing Address: P.O. Box 745. Colorado Springs, Colorado 80235 Telephone (303) 598-5830

29 May 1974

Transportation Systems Center Kendall Square Cambridge, Maine 02142

Attention: TCD

Gentlemen:

Attached is a description of our dispersion model used to calculate 275 cases of highway carbon monoxide pollution from input data furnished by TSC, in accordance with Order No. TS-8153, 28 March 1974, Requisition No. TCD-5157.

Also attached are listings of the TSC input and KSC output. The output is being shipped separately on punched cards. Calibration test case results are not included because they were not run.

In this task we used 81 man hour: of Scientist/Programmer at $9.70~\mathrm{per}$ hour.

One comment we wish to make about the program pertains to emission factors. Only traffic counts and speeds were given, not the mix of automobiles of different yearly vintages. This meant that results could differ because of differing assumptions about the mix of automobiles.

I hope this satisfies your requirements. We were pleased to participate in this study and look forward to further activities with TSC.

Sincerely,

Wm. J. Veigele, Manager Environmental Programs

WJV:kr Enclosures SYSTEMS CONTROL, INC. 1801 PAGE MILL ROAD PALO ALTO, CALIFORNIA 84304

TELEX | 348433

Tecemoire (116) 494-1161

May 17, 1974

Mr. Paul Downey
U. S. Department of
Transportation
55 Broadway
Kendall Square
Cambridge, Mass. 02142

Subject: Task Order TS-8142

Paul:

With reference to this task order, and our phone conversation 16 May 1974, enclosed are the required data cards that delineate the results of this model prediction study. If you have any questions, please do not hesitate to call me or Ron Lau (415-494-1165).

For your future reference our company has moved to the following new address:

Systems Control, Inc. 1801 Page Mill Road Palo Alto, California 94304

A full description of SCI's model and assumptions used in this study will be sent to you as soon as possible. It should be noted, in general, that the specific lata base specified by TSC (for the highways under consideration) required modification of SCI's standard models for the proper response to the objectives of this study.

Have a pleasant day,

Rolf & Schainka

Dr. Robert B. Schainker

RBS: kt

cc: Ms. Ruth E. Chandler U. S. Dept. of Transportation 55 Broadway Kendall Square Cambridge, Mass. 02142



SYSTEMS, SCIENCE AND SOFTWARE

May 9, 1974

SSS-R-74-2234 Ref.: WO 262

Mr. Paul J. Downey Transportation Systems Center Kendall Square Cambridge, MA 02142

Reference: TCD

Dear Mr. Downey:

Systems, Science and Software (S³) herewith submits its results for the Transportation Systems Center (TfC) dispersion model validation experiments. Under separate cover we are sending punched cards with the S³ predicted concentrations in ppm for each case for all three sites. In addition, we are enclosing a brief discussion of our model, EXPLOR, and a graph showing the emission factors we used for each site.

Sis model requires an emission factor as input. We used a standard set of values for 1972 and 5% heavy outy traffic. All validation runs were made with these values, then the predicted concentrations without background were least squares fitted to the measured concentrations less background. From this a factor was obtained to translate the curve, as shown, for each site. It would be helpful on future studies if emission factors were supplied so that all codes being evaluated used a standardized set. In that way, the codes could better be evaluated on how well they handled the physics of the problem.

S³ directly added the background concentrations supplied at each level to the EXPLOR predicted downwind concentrations at the appropriate level for sites 11 and 14. For site 15, S³ added the given background concentration directly to each downwind predicted value at whatever level.

S⁹ was pleased to take part in this study and would be happy to participate in any future validation studies you anticipate running. Our code is capable of handling quite complex topography so we would particularly enjoy a validation study where terrain is critical.

P.O. BOX 1620, LA JOLLA, CALIFORNIA 92037, TELEPHONE (714) 453-0060

May 4, 1974

Mr. Paul J. Downey

We will be very interested in your evaluation results when they are completed.

If you have any questions about our code or results, planse do not hesitate to call.

Sincerely,

Ruth S. Sheridan

Environmental Sciences Dept.

RSS:bz

Enclosures

APPENDIX E. MODEL VALIDATION STATISTICS

MODEL VALIDATION STATISTICS

Peter H. Mongert David S. Prerau Transportation Systems Center

1.0 INTRODUCTION

This report deals with the statistical techniques to be incorporated in the DIspersion MOdel TEst (DIMOTE)* package. It considers various possible tests for comparing air pollution dispersion models with regard to their usefulness in predicting pollution based on known, or estimated, pollution sources and other attendant physical factors. The term "model" here refers to a specific computer program accepting standard inputs from the DAta REtrieval System (DARES)* and predicting pollutant concentrations at specified places and times according to the format of the Standard Model Output Generator (SMOG)*. Because they accept standard common inputs and give outputs relating to common concentration estimations, the models can be compared if actual concentration measurements were made at the points where the pollutant concentration is estimated by the models.

The report will cover the following topics:

- I. Description of types of experimental data to be used and the general nature of the comparison of the models.
 - II. Purposes and desired properties of the models.

^{*}DIMOTE, DARES and SMOG are computer routines of the Transportation Air Pollution Studies (TAPS) System which is described in Interim Report No. DOT-TSC-OST-73-24, The Transportation Air Pollution Studies (TAPS) System by David S. Prerau and Paul J. Downey, June 1973.

- III. The types of tests which can compare the models according to their expected use. This is the heart of this report and will get the most complete treatment.
 - IV. Discussion of the arbitrariness in selecting tests.
- V. Discussion of the problem of "tuning" models on the test data and comparing models on the same data.

2.0 OVERVIEW OUTLINE

- As The information coming from the models is used to make decisions.

 Hence, all tests to be proposed will measure directly, or indirectly, the usefulness of the model as an aid in correct decision-making.
- B. One approach to test-construction is to anticipate the types and relative frequencies of decisions, how the decision will be made using the model (the decision function) and how well the model will perform, i.e. the probability of its leading to correct decisions. The factors leading to wrong decisions combine to give an expected loss using each model that πodel is favored which gives the least expected loss. This will be referred to as the Decision Theoretic Approach.
- 1. Some of these factors must be estimated from a priori knowledge and experience and even "educated guesses." This is a fact of life of Bayesian (See p.7) decision theory and considered preferable to completely arbitrary methods with perhaps elegant structure but ignoring the expected use to which the information is to be put in making decisions.
 - 2. Other factors of course may be estimated from the test experimental data -

this is the manner in which the experiment discriminates between the models.

- a. Specifically, when a decision function is known, the probabilities of wrong decisions can be estimated from the experimental data collection to test the models.
- b. Even the decision function can be chosen using the experimental data that decision function leading to the least expected loss for that model would be chosen. This amounts to "tuning" the model, i.e. perhaps expecting lower or higher pollutions than the model explicitly predicts.
- C. Alternatively, one can estimate the performance in decision situations by qualitatively constructing loss functions which increase as the predicted values deviate more from the measured values or as the predicted values show less of a tendency to increase with measured values. This approach will be discussed in the section on Other Measures.
- 1. One can construct intuitive loss functions which indicate various average measures of deviation of predicted values from measured values
- a. One of the simplest and oldest but probably not very useful in this application - is the sum of the squares of the deviations:

 $\Sigma(C_i-\hat{C}_i)^2$

 $\mathbf{C}_{\hat{\mathbf{I}}}$ and $\hat{\mathbf{C}}_{\hat{\mathbf{I}}}$ are respectively the measured and predicted values for the ith point in space and time.

Others selected for various desirable properties could be quite useful. For example:

$$\Sigma a_i C_i^{\alpha} (\log C_i - \log \hat{C}_i)^2$$

has useful properties which will be discussed in Chapter 5.

- 2. Other measures are of interest; for instance loss functions which measure the tendency of the predicted value to increase with the measured value. This can be of value in selecting models with respect to their ability to predict increases in pollution under certain circumstances. A full blown decision theoretic approach is possible along the lines indicated in B above and to be described in more detail later. Alternatively, a simple correlation coefficient is sometimes useful. However, we do not especially recommend the standard correlation coefficient for this purpose because of the assumption of linearity on which it is based. The rank correlation coefficient would be useful, however.
- 3. Tests which do not refer each predicted value specifically to its corresponding measured value (i.e., which ignore the inherent pairing of predicted and measured values) must be specifically avoided. This includes measures of how well the distribution of predicted values matches the corresponding distribution of measured values. Such tests can always be replaced by more informative and powerful tests and can give misleading results because they ignore information quite needlessly. In particular, along these lines, the Kolmogorov-Smirnov test which is quite powerful in its proper place would be of minimal usefulness in this context.

3.0 DECISION THEORETIC APPROACH

A model will be used to make decisions. We will analyze a simple "go/no-go" decision. The model will be used for a complex linear mix of such binary decisions and the analysis of the simple decision will form the foundation for showing how the model is to be tested for its value in making decisions. Suppose a concentration level C_{S} is set as a standard. If the pollution exceeds $\mathbf{C_S}$ then one action is preferred, while if it falls below $\mathbf{C_S}$, some other action is preferred. We shall call these actions the high pollution and low pollution actions, respectively. If we make the high pollution action, then we have made the high pollution decision and vice versa. The high pollution action might be to not build something which is a potential source or to not operate something which is a potential source; the low pollution action would be the reverse. If the pollution exceeds $C_{\rm g}$ and we make the low pollution decision (take the low pollution action), then we incur a loss \mathbf{L}_1 relative to making the right decision. If the pollution is below $\mathbf{C}_{\mathbf{S}}$ and we make the high pollution decision our loss is ${\bf L_2}.$ The model will predict a pollution $\hat{\bf C}.$ A decision function D must be selected. It takes the form:

 $\label{eq:condition} \text{if $\hat{\mathbb{C}}$>C_d, decide high pollution (i.e. C^C_s); if $\hat{\mathbb{C}}$<C_d, decide low pollution (i.e. C^C_s) where C_d is to be calculated as shown below.}$

If we know the a priori distribution of \hat{C} , Pr(C), and the conditional distribution of C given \hat{C} , Pr(C>C_S| \hat{C} = \hat{C}_2), we can estimate the loss as:

$$L = L_1 \cdot \int_{-\infty}^{C_d} \Pr(C > C_s \mid \hat{C} = C_2) \Pr(C_2) dC_2 + L_2 \int_{C_d}^{c_0} \left[1 - \Pr(C > C_s \mid \hat{C} = C_2) \right] \Pr(C_2) dC_2$$
 (1)

Cd is chosen to minimize this expected loss.

The above determination of C_d is what we refer to as "tuning" the model in this particular case. If the model were perfect and always predicted the correct measured pollution, C, then $C_d = C_S$ would be the correct choice. However, even if the model is quite good and unbiased C_d will differ from C_S if the ratio of L_1 to L_2 is substantially different from unity, thereby forcing conservative decisions to be made (e.g. decide $C > C_S$ even if it probably isn't, because L_1 is so much greater than L_2). In other words, the decision level for the model may be different (usually less than) the concentration standard level.

The main constituents in equation 1 are of the form:

- 1. $Pr(C>C_1|\hat{C}=C_2)$
- 2. Pr(C2)
- 3. $L_1 L_2$

The estimation of these quantities will now be discussed.

The conditional probability $\Pr(C>C_1|\hat{C}=C_2)$ is to be estimated from the experimental data. In fact it carries all the information in the experimental data bearing on the relative suitability of the model. In the parlance of statistics, $\Pr(C>C_1|\hat{C}=C_2)$ is a "sufficient statistic" for selecting a model (it is of course not a single number, the value must be known for all C_1 , C_2). The estimation of these conditional probabilities will be discussed in the next section.

Tables of these conditional probabilities will be constructed, as they can be used in constructing decision functions and evaluating models for situations not yet envisioned.

The a priori distribution $Pr(C_2)$ must be estimated in the presence of uncertainty. It would be based on an estimate of the a priori distribution of the model inputs. This would then imply an a priori distribution of the model output, for each specific model. The a priori distribution of inputs comes from the expected strengths and other attendant conditions expected in general usage of the model in making the type of decision under consideration. This estimate does not refer to specific model inputs or to any observed pollution levels. Thus, our ignorance of this function is usually not serious; the more precise information is carried in the conditional distribution, $Pr(C>C_1 | \hat{C}=C_2)$.

Note that only the ratio of L_1 to L_2 is needed in both choosing the decision function and in discriminating between two models (See equation 1). The ratio is ordinarily much easier to guess than the absolute (dollar) values of L_1 and L_2

The models will ordinarily be expected to be used in numerous decisions. Each will have its decision function optimized and then the total expected loss will be the sum of the expected losses in the individual cases, each weighed by its expected frequency. Again we have several quantities to estimate with few known facts to estimate them on. This is the nature of Bayesian decision theory*: it gives an objective framework in which to imbed unavoidable subjective estimates.

^{*}Bayesian decision theory derives from "Bayes' rule", which assigns a posteriori probabilities to events based upon empirical observation and a priori probabilities. Since there is often no analytic method to know the a priori probabilities required, they must in effect be replaced by reasonable guesses.

4.0 THE CONDITIONAL DISTRIBUTION FUNCTION

As we said above, the conditional distribution function, $\Pr(C > C_1 | \hat{G} > C_2)$, (the probability that the measured value will exceed C_1 given that the model predicts C_2) contains all the information derivable from the proposed experiment which is germane to discriminating between models.

There are various ways to estimate this function from an experimental data set (i.e. the pairs C_i , \hat{C}_i , i=1,...,N). All are subject to statistical error due to the finite sample size, N. This will be especially true if we ascribe importance to values of C which are sparsely represented in the data set (e.g. high pollution levels which occur quite infrequently in the experimental data). There seems to be no good way around this. In general, data cannot be reliably extrapolated into regions where measurements are not taken. If it can be known confidently that a model which has a certain percent error at one pollution level will have the same percent error at a different pollution level, then this extrapolation may be possible. In any case, the best characterization of data bearing on the conditional distribution is probably the Natural Histogram in the case where it can safely be assumed that the measured value increases with the predicted value. This approach will be described below and its properties discussed. The Natural Histogram provides an estimate of the conditional distribution function which can aid the Planner in choosing a model suitable for his application.

In order to obtain a good estimate of the conditional probabilities $\Pr(\text{C} {>} \text{C}_1 \, | \, \hat{\text{C}} {=} \text{C}_2)$

the Natural Histogram is used. The Natural Histogram is considered to be the "minimal sufficient statistic" for estimating the conditional probabilities from experimental data.

As shown by the example in Figure 1, the Natural Histogram is a monotonic step function which, for a given C_1 , gives the probability that the measured concentration is greater than C_1 for each value of the predicted concentration, C_2 . Note that the Natural Histogram consists of a set of intervals or "steps" in which the estimated probability is constant. For each such interval of C_2 , this estimate is equal to the empirical frequency of the event $C > C_1$ within that interval. The intervals are chosen to be the minimum size consistent with monotonicity.

The algorithm for choosing the intervals and determining the estimated probability for each interval is shown in Figure 2. The data points are ordered by their predicted values, \hat{C} . Then, each of the entries on the corresponding list of reasures values, C, is compared with the given level, C_1 . The flowchart shows how the probability P(s) and the size, T(s), of each step, s, of the Natural Histogram is then found.

5.0 OTHER MEASURES TO USE IN DISCRIMINATING BETWEEN MODELS

Besides the statistical approach which we have briefly presented, there are other

(far simpler) measures of how well the predictions of the model match the measures

or actual pollution. These measures do not in general extract the invariant information from the experiment; they are influenced more than necessary by the choise of

pollution levels at which the experiment is run. Furthermore, they make no attempt

to match the measure as closely as possible to the intended usage of the model.

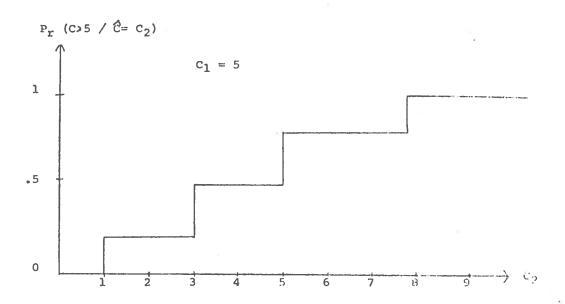
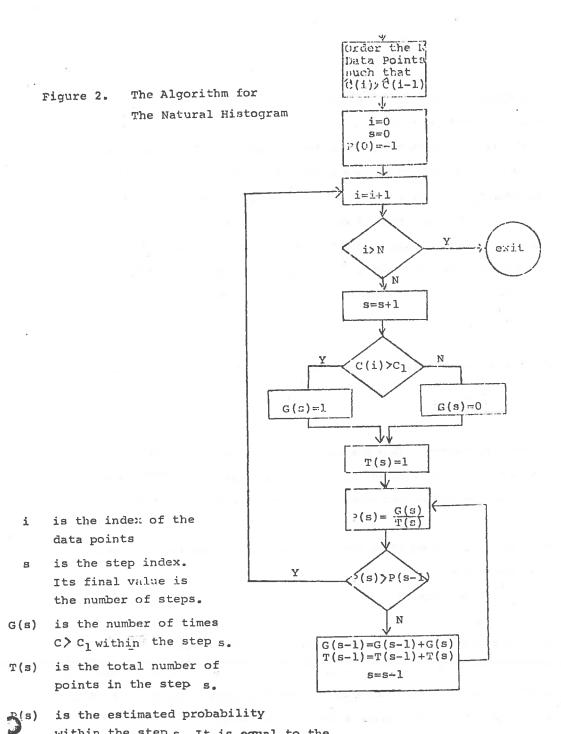


Figure 1. An example of the Natural Histogram



within the step s. It is equal to the empirical frequency $\frac{G\left(s\right)}{T\left(s\right)}$.

Nevertheless, because these approaches are direct and simple they should be applied, since the cost is small and the potential usefulness of the results is significant. Furthermore, since the approach is simple and intuitive, it is sometimes possible to discover aspects of the correlation between measured and predicted concentrations in this way which are not revealed by the previously discussed statistical framework which has its own limitations. In addition (again because of the simplicity of these measures), it will sometimes be possible to derive and estimate a statistic which measures the statistical significance of the observed difference between the models - a definite benus in those cases where it exists.

For the purpose of illustrating such measures, consider the familiar one:

$$L_{=\frac{1}{N}} \int_{i=1}^{N} (C_{i} - \hat{C}_{i})^{2}$$

the mean square error. This measure would only be used if it had become a standard measure for other workers in the area. However, its properties don't hold here and in fact accrue to a related measure which we now discuss.

Since the percent error of the prediction is of more importance than the absolute error, the measure

$$L_{=} \sum_{i=1}^{N} (\log C_{i} - \log \hat{C}_{i})^{2}$$

is of particular interest. It has at least two other important factors in its favor.

1. Some models predict the pollution to be proportional to the inputs. In so far as this is an invariant fact, the percentage error of the model should be a constant for the entire range of concentration levels.

2. Air pollution distributions have been postulated to be log normal.

The sum of the squares of the differences in logs is a selected and favored statistic for such a distribution.

The measure:

$$L = \sum_{i=1}^{N} (\log C_1 - \log \hat{C}_i)^2$$

is useful but it may be necessary to modify it to accentuate those regions where model performance is most critical. Specifically,

$$\begin{array}{l} \textbf{L=} \ \ \textbf{E} \ \ \textbf{a}_{i} \ \textbf{b}_{i} \ \ \textbf{C}_{i}^{\alpha} (\log \textbf{C}_{i} - \log \hat{\textbf{C}}_{i})^{2} \\ \\ \textbf{a}_{i} = \textbf{A} \ \text{if} \ \textbf{C}_{i} > \hat{\textbf{C}}_{i} \\ \\ \textbf{a}_{i} = \textbf{a} < \textbf{A} \ \text{if} \ \ \textbf{C}_{i} < \hat{\textbf{C}}_{i} \end{array}$$

b_i is chosen as a weight representing the estimated significance or importance of the ith experimental pair. The b_i's will ordinarily be equal in blocks with certain blocks of data from the experiment being favored over others with respect to reliability, relevance, range of values, etc. a_i depends on whether the measured value exceeds or is less than the predicted value. Over-predicting may be less serious than under-predicting.

The factor \mathcal{I}_{i}^{α} represents our assessment that the performance of the model is more important at high pollution levels than at low pollution levels. In fact, if the pollution level is very low, not only is the prediction of little interest practically, but the pollution from the selected sources may be oversnadowed by that from exogenous sources. For practical purposes $\alpha=1$ seems to be a suitable value, though other α values can be tried.

A general loss function may be found of the form

$$L = \sum b_i R(C_i, \hat{C}_i)$$

where again b_i is a significance weighing for the ith experimental pair and R is a function which increases as its two arguments, C_i , \hat{C}_i , get farther spart. Let us denote the term b_i $R(C_i,\hat{C}_i)$ (which includes $a_ib_iC_i(\log C_i - \log \hat{C}_i)$) as a special case) by S_i and let its dependence on the model, labeled by j, be expressed by S_{ij} (b_i and the functional form of R do not depend on the model, nor does C_i , but \hat{C}_i does.) We now may write:

$$L_{j} = \frac{1}{N} \stackrel{N}{\stackrel{\Sigma}{=}} S_{ij}$$

as the loss function for the j th model. Suppose $L_2>L_1$, indicating that model 1 may be better than model 2. We may wish to test the statistical significance of this conclusion, i.e. test the hypothesis: $\langle L_2 \rangle - \langle L_1 \rangle > 0$ where the " $\langle L_2 \rangle - \langle L_1 \rangle > 0$ brackets denote expected value (i.e. the true mean value).

Let
$$S_j^2 = \frac{1}{N-1} \sum_{i=1}^{N} (S_{ij}^{-L}_j)^2$$

Then

$$t = \frac{L_2 - L_1}{S_1^2 + S_2^2}$$

may be referred to Student's t-tables at the appropriate level of significance with the appropriate number of degrees of freedom. The resultant probability is a confidence level for the significance of the difference between two models, as indicated by this measure. If the process is indeed log normal and $S_i = (\log C_i - \log \hat{C}_i)^2$ then all the 2N-2 possible degrees of freedom may be used. If these assumptions do not apply then fewer degrees of freedom are applicable which is not so favorable. In general it must be concluded that a precise estimate of the relevant number of degrees of freedom will be difficult. This

is true in many practical situations. However, if reasonable circumstances prevail (which can be determined from the loss function used and pertinent statistics which the constituent quantities follow) and if there is a sufficient number of measurements, then the number of effective degrees of freedom is infinite. This will ordinarily be the case if over 100 measurements, C_{i} , are taken. In this case, the probabilities may then be determined and the hypothesis tested without difficulty.

Other intuitive measures are not expressible in the form $L=\Sigma S_{ij}$. For example, it may be of interest to determine the tendency of larger predicted values to be associated with larger measured values, independent of the absolute accuracy of the prediction. Here, a rank correlation measure may be used. The rank correlation coefficient may be defined as follows:

Let the \hat{C}_i , i=1N be ordered into the sequence $\hat{C}_{(1)}$, $\hat{C}_{(2)}$ \hat{C}_R Similiarly, rank the sequence C_i , i=1 ..., N. Let the i th ranked C be paired with the j th ranked \hat{C} . The sum Σ i.j is called the rank correlation coefficient. As stated, in this summation, i represents the ranks of a C and j the rank of the corresponding \hat{C} , when the C's are ranked together and the \hat{C} 's are ranked together. The rank correlation coefficient is called a "non-parameteric" measure of the tendency of the variable C to be an increasing function of the variable \hat{C} (and vice versa). It measures the desirable property of having the measured pollution being an increasing function of the predicted pollution. This is a very important property.

Still other measures of model validity could be proposed. It must be cautioned however, that not every measure with intuitive appeal is acceptable for this purpose. If the measure disregards too much information contained in the experimental data (such as is true of tests based on the distribution of C and \hat{C} , separately), it may have little validity. The tests we have described in this report should be adequate for testing models. Other tests will be included if appropriate.

6.0 DIMOTE TEST PLAN

DIMOTE will compute a set of statistics from the results of the test runs made with each air pollution dispersion model. Initially, the following statistics will be calculated:

- 1. Log Difference Squared Loss Function
- 2. Biased Log Difference Squared Loss Function
- 3. Rark Correlation Coefficient
- 4. Natural Histogram

The Log Difference Squared Loss Function, LDS. is defined by:

$$LDS = \sum_{i=1}^{N} (log\hat{C}_i - logC_i)^2$$

where $C_{\hat{\mathbf{1}}}$ is the ith measured pollutant concentration value $\hat{C}_{\hat{\mathbf{1}}} \text{ is the corresponding value predicted by the model}$ N is the number of measured values

A second loss fraction will also be used. This is the Biased Log Difference

Squared Loss Function, BLDS, which is defined by;

BLDS =
$$\sum_{i=1}^{N} \beta_i C_i (\log \hat{C}_i - \log C_i)^2$$

where $\mathbf{C_i}_{,}\mathbf{C_i}_{,}$, N are as defined above and $\boldsymbol{\beta_i}$ is defined by:

$$\beta_{i} = 1 \text{ if } \hat{C} > C_{i}$$

$$\beta_{i} = 2 \text{ if } \hat{C}_{i} < C_{i}$$

In this loss function, the log difference squared is weighted by $C_{\hat{i}}$ (to give greater weight to higher concentration values) and by $\beta_{\hat{i}}$ (to give greater penalty to underprediction than to overprediction).

The Rank Correlation Coefficient will be the third statistic computed for each model. This will be found by the following technique:

- 1. The measured values and corresponding predicted values are listed in ϵ 2xN matrix.
- 2. The measured values are ordered, carrying the corresponding predicted values with them.
- 3. Each measured value is replaced by its rank number (the lowest measured value is replaced by 1, the next lowest measured value by 2, etc.).
- 4. The predicted values are then ordered, carrying the corresponding measured value ranks with them.
 - 5. The Rank Correlation Coefficient, R, is found by

$$R = \sum_{j=1}^{N} (r_{j}-j)^{2}$$

where r_i is the measured value rank number of the jth pair as ordered in Step 4.

The fourth computation performed by DIMOTE for each model is the computation of the Natural Histogram. From the Natural Histogram, one hundred values are computed. Ten levels, C_k , are defined by:

$$C_k = C_L + k \cdot \frac{C_{11} - C_{1}}{11}$$
 $k = 1, 2, ..., 10$.

where C_{L} is the lowest measured value

 $C_{\mathbf{H}}$ is the highest measured value

For each level, ten conditional probabilities are computed:

$$\begin{aligned} & P_{\mathbf{r}}(C > C_{k} | \hat{C} = \hat{C}_{j}) \\ & \text{for } \hat{C}_{j} = \hat{C}_{L} + j \frac{\hat{C}_{1j} - \hat{C}_{1}}{11} \quad j = 1, 2, \dots, 10. \end{aligned}$$

where \hat{C}_L is the lowest predicted value $\hat{C}_H \text{ is the highest predicted value}$

7.0 TAPS VALIDATION REPORT FORMAT

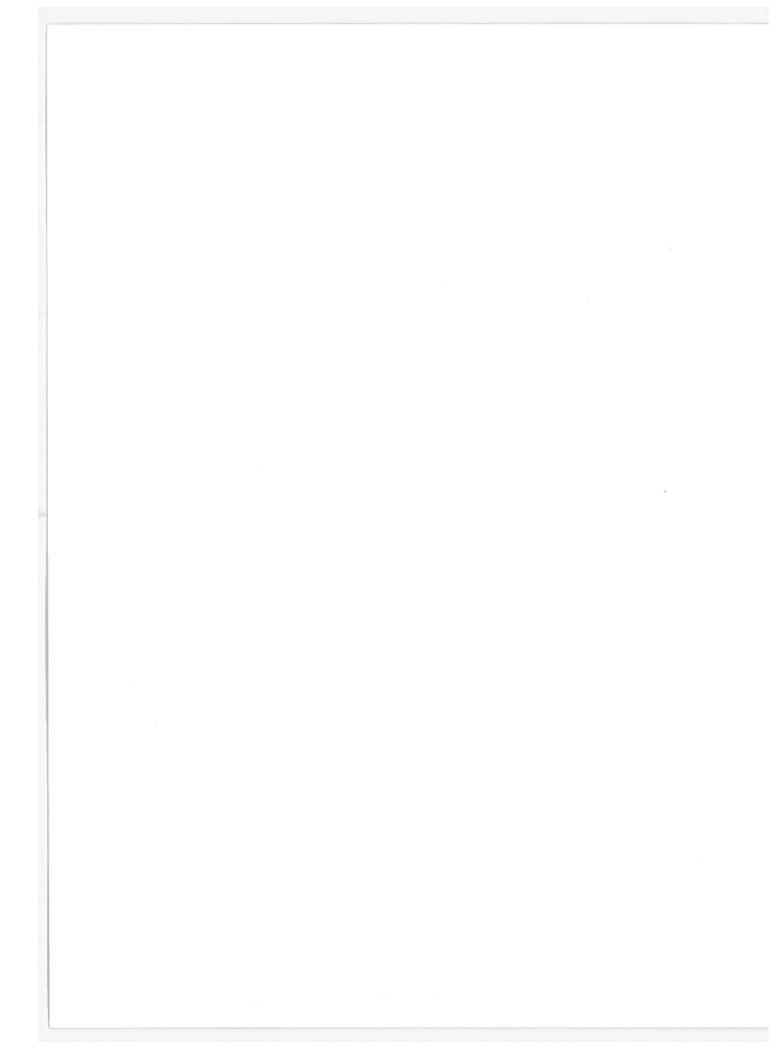
A final TAPS Validation Report, as now envisioned, will consist of the following four sections:

 $\underline{\textbf{Section 1: Introduction}}. \label{eq:section will discuss the background of TAPS and it; goals. This section will be similar in each TAPS Report.$

Section 2: Discussion of Statistics. This section will be similar to the statistical discussion in this report and will explain each of the tests used by DIMOTE. It will also discuss the use of the DIMOTE output data. This section will also contain sample usages, as well as warnings to the user as to limitations of the statistics. The discussion here will be similar in each TAPS Report, changing as new statistical tests, or outputs, are added to DIMOTE.

Section 3: Model Statistics: This section will contain tabulations of the statistics calculated for each model. These will initially include the four statistics named above. In addition, it will include other model descriptors such as average model run-time, amount of data necessary for model usage, usuability of model with missing data, ease of the use, etc.

<u>Section 4: Model Comparisons</u>: This section will present tables and graphs which will enable the user to compare the tested models with respect to his own decision problem. Tables of comparative loss functions and rank correlation coefficients will be included.



APPENDIX F. CORRESPONDENCE FROM THE WASHINGTON DC DEPARTMENT OF HIGHWAYS AND TRAFFIC

GOVERNMENT OF THE DISTRICT OF COLUMBIA DEPARTMENT OF HIGHWAYS AND TRAFFIC

ADDRESS REPLY TO
OFFICE OF PLANNING & PROGRAMMING
415 - 12th STREET, N. W.
WASHINGTON, D. C. 20004



July 1974

Mr. Paul J. Downey Transportation Systems Center Kendall Square Cambridge, Massachusetts 02142

Dear Mr. Downey:

This is in response to our telephone conversation yesterday regarding cross sectional dimensions for roadways used in data collection in developing the Motor Vehicle Pollution Simulation Model. The dimensions for Independence Avenue were scaled from aerial photography. There are six lanes, but the total roadway width is 68 feet rather than 72 feet as shown. In addition, I have verified that the center strip width at the monitoring point is 45 feet (apparently, we had a scaling or typographic transcription error to indicate 95 feet).

I have also reviewed the other dimensions shown and find dimensions for the Southwest Freeway which might be misleading to you. The total number of lanes and pavement width appear to be correct, but the center strip width seems to reflect only one of the several divider areas. The out-to-out dimension of readway including median, pared lanes and shoulders scales from contract drawings at 220 feet. This includes two 10 foot shoulder spaces and paved divider moses. The 270 foot divension for the cut section is correct.

I hope that this data coupled with the sketches in the final report will be sufficient for you to validate the model prior to application in Massachusetts.

Sincarely yours,

LICHARD A. DeMAST Assistant Director

INDEPENDENCE AVENUE

Number of Lanes: 6

Highway Width: 72' (6-12' lanes)

Center Strip Width: 95'

WHITEHURST

Number of Lanes: 4
Highway Width: 48' (4-12'lanes)

Center Strip Width: 4':

E Street

Number of Lanes: 4

Highway Width: 40' (4-10' lames)

Center Strip Width: 10' Width of Cut: 60' Depth of Cut: 25'

MILITARY ROAD

Number of Roses: 4

Highway Width: 52' (4-13' lanes)

Center Strip Width: 6'

ANACOSTIA

Number of Lames: 4

Highway Width: 48' (4-12' lones)

Centur Strip WM Cth: 431

Height of Road Above Ground: 25'

SOUTHWEST PREEMAY

Number of Lames: 11 6 lames main roadway, 5 ramp lames

Highway Width: 132' (11-12' lames)

Center Strip Width: 40' Width of Cur: 270' Depth of Cur: 24'

NOTE: Highway width equals width of roadways only. For curb to curb measurement add center strip width.

MOLEL VALIDATION RESULTS - INDEPENDENCE AVE (SITE 11) VALUES MEASURED DURING SEPTEMBLE 27:1972 - OCTOPER 14:1972

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MOLEL VALIDATION HESULTS - INDEFENDENCE AVE (SITE 11)
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MOLEL VALIDATION RESULTS - INLEPENDENCE AVE (SITE 11)
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MOLEL VALIDATION RESULTS - INLEPENDENCE AVE (SITE 11) VALUES MEASUREU DURING SEFTEMBER 27,1972 - OCTOFER 14,1972	
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RODEL VALIDATION RESULTS - MILITARY ROAD (SITE 14) VALUES MEASURED DURING SEPTEMBER 27,1972 - OCTOBER 14,1972

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MODEL VALIDATION RESULTS - MILITAN ROAD (SITE 14) VALUES MEASURED DUHING SEPTEMBER 27:1972 - OCTORER 14:1972

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MODEL VALIDATION RESULTS - MILITA... ROAD (SITE 14)
VALUES MEASURED DURING SEPTEMBER 27:1972 - OCTOBER 14:1972

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MODEL VALIDATION RESULTS - MILITARY ROAD (SITE 14)
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MODEL VALIDATION PESULTS - MILIT. 17 ROAD (SITE 14) VALUES PLASURED DURING SEPTEMBER 27:1972 - UCTORER 14:1972

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