A CRITICAL REVIEW
OF
MATHEMATICAL DIFFUSION MODELING TECHNIQUES
FOR
AIR QUALITY
WITH RELATION TO MOTOR VEHICLE TRANSPORTATION

A Study
Prepared for the

WASHINGTON STATE HIGHWAY COMMISSION
DEPARTMENT OF HIGHWAYS

by

Donna V. Lamb
Franklin I. Badgley
August T. Rossano, Jr.

University of Washington
Departments of Atmospheric Sciences
and Civil Engineering
Seattle, Washington

June 1973

A CRITICAL REVIEW OF MATHEMATICAL DIFFUSION MODELING TECHNIQUES FOR PREDICTING AIR QUALITY WITH RELATION TO MOTOR VEHICLE TRANSPORTATION

by

Donna V. Lamb, Franklin I. Badgley, August T. Rossano, Jr.
Departments of Atmospheric Sciences and Civil Engineering
University of Washington
Seattle

ABSTRACT

At the request of the Washington State Department of Highways a literature review was undertaken to assess the state-of-the-art in air quality modeling as related to motor vehicle transportation problems. In addition to reviewing the published literature, several private companies and governmental agencies with available models were contacted as were individuals working in the field. Models which were available for review are described and examined with respect to identification of latest state-of-the-art characteristics, model applicability, and limitations. Recommendations on the use of air quality diffusion models are offered.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

1.0 PROJECT STATEMENT AND OBJECTIVES

Federal and State laws require highway departments to prepare statements assessing the impact that proposed highway improvements or construction may have on the environment. An important consideration in the preparation of an impact statement is the anticipated effect the proposed activity will have on air quality since highway transportation is a source of several major air pollutants: particulate matter, nitrogen oxides, carbon monoxide, hydrocarbons, and photochemical oxidants which are formed in the atmosphere in the presence of sunlight. Comprehensive physical studies to predict the air quality impact at proposed sites are generally prohibitive due to the time required to obtain suitable data, the cost of such studies and the number of impact statements that must be considered by most highway departments.

Methods have been developed to predict the air quality impact of new highway construction through the use of mathematical atmospheric diffusion models. Once they are properly calibrated these models can be used to test alternative locations and designs. Basically models use meteorological conditions and emission rates to predict downwind concentrations as illustrated in Figure 1.

The principal objective of this research project has been to conduct a search of the literature to identify state-of-the-art air quality predictive schemes applicable to motor vehicle transportation. The available models have been analyzed in detail and evaluated in terms of selected characteristics that serve to describe the predictive capabilities of each. Limitations in the models have also been noted where appropriate.

Section 2.0 of this report describes the methods used in conducting the research. Sections 3.0 and 4.0 present the models analyzed and a

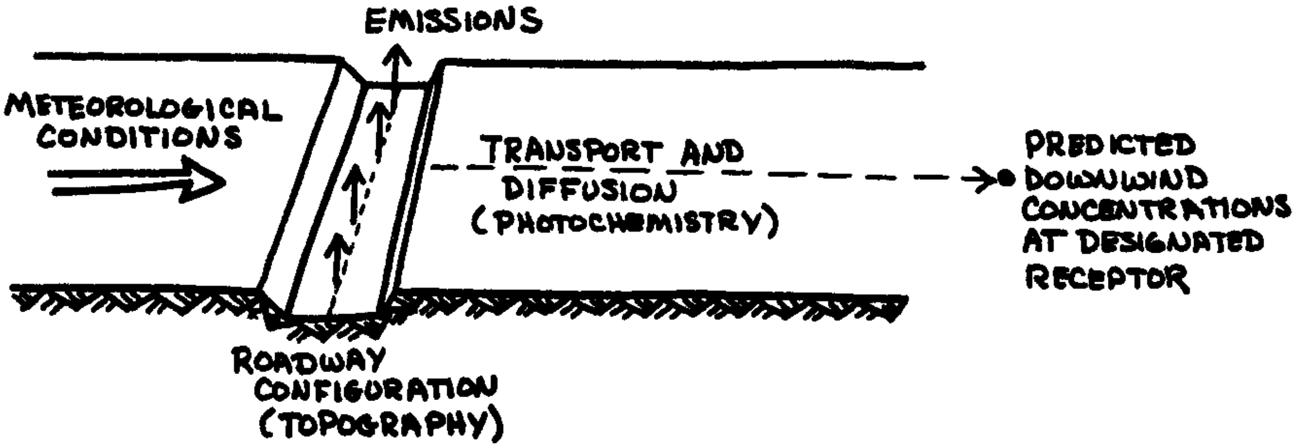


Figure 1. Role of models in relating emissions, meteorological conditions and other factors to air quality concentrations.

general discussion of applicability, in both narrative and tabular form. Section 5.0 summarizes the study and presents the recommendations for future consideration.

2.0 METHOD OF ANALYSIS

The Washington State Highway Department provided a copy of the U. S. Department of Transportation (DOT) Report on "Computer Modelling of Transportation - Generated Air Pollution." As an initial effort, this report was reviewed to ascertain if it was a sufficient survey of the state-of-the-art in modeling to meet our purposes. It was concluded that although the report serves as a good general survey, the descriptions of available models are not complete enough to serve as a basis for making recommendations or identifying state-of-the-art. Furthermore, some models of importance were not mentioned in the DOT report.

Using the DOT report as a starting point, specific details regarding selected models were requested (via letter) from companies or organizations that appeared to have made significant contributions or refinements in existing techniques. In addition, experts working in the field as well as governmental officials were contacted to assess recent modeling developments and model validation studies.

Table 1 presents a list of names and addresses of companies and individuals contacted and the results of that contact. Various air pollution abstracts were searched as well as primary journals in the fields of air pollution and atmospheric sciences. Many of the papers were found in the proceedings of various symposia that have been held in the last few years. The models reviewed in this report are primarily new models developed in the last two or three years. Time did not permit review of the older models which led to the development of current models.

Four persons were interviewed: Jerry Kurtzweg and Dean Wilson of the Seattle Office of the Environmental Protection Agency (EPA), Francis Ludwig of the Stanford Research Institute, and Andrew Ranzieri of the

California Highway Department. They were most helpful in suggesting important models to consider and important people to contact. Information obtained in these interviews is interspersed throughout this report.

Table 1. List of persons contacted.

Name and Address	Contacted by	Response	Particular reason for contact
Aerovironment 660 South Arroyo Parkway Pasadena, California 91106	Letter	Brochure, several papers and reports	
Kenneth L. Calder Division of Meteorology, EPA Research Triangle Park, North Carolina 27711	Letter	-	
E. J. Croke Center for Environmental Studies, Building 12 Argonne National Laboratory 9700 S. Cass Avenue Argonne, Illinois 60439	Letter	Several papers and letters	
Environmental Research and Technology, Inc. 429 Marrett Road Lexington, Massachusetts 02173	Letter	-	Interesting parameterization of the wind-field included in a Gaussian model
A. Q. Eschenroeder General Research Corporation P. O. Box 3587 Santa Barbara, California 93105	Letter	Several papers and letters	Has been working on photochemical models for some time. Papers are not available in open literature.
ESL, Inc. 495 Java Drive Sunnyvale, California 94086	Letter	Letter, papers	

Table 1 (continued)

Name and Address	Contacted by	Response	Particular reason for contact
GEOMET, Inc. 50 Monroe Street Rockville, Maryland 20850	Letter	-	Working in the area of photochemical modeling - one model being investigated by EPA
Steven R. Hanna Atmospheric Turbulence and Diffusion Laboratory NOAA, P. O. Box E Oak Ridge, Tennessee 37830	Letter	Several papers	
INTERCOMP Resource Development and Engineering, Inc. 200 West Loop South Suite 2200 Houston, Texas 77027	Letter	Letter, several papers	
Joseph B. Knox Atmospheric Science Group, Lawrence Livermore Laboratory University of California P. O. Box 808 Livermore, California 94550	Letter	Several papers	
Jerry Kurtzweg Environmental Protection Agency 1200 Sixth Street Seattle, Washington 98101	Interview	Several papers	
Robert G. Lamb Department of Chemical Engineering California Institute of Technology Pasadena, California 91109	Letter	Letter, several papers	

Table 1 (continued)

Name and Address	Contacted by	Response	Particular reason for contact
Peter Loux Computer Science Co. 1701 N. Fort Meyer Drive Arlington, Virginia 22209	Letter	-	Person to contact about non-EPA use of UNAMAP
Francis L. Ludwig Stanford Research Institute Menlo Park, California 94025	Interview Letter	Several papers on SRI models, current research	
Meteorology Research, Inc. 464 West Woodbury Road, Box 637 Altadena, California 91001	Letter	-	Model is being tested by the California Highway Department group
L. O. Myrup Department of Agricultural Engineering University of California at Davis Davis, California 95616	Letter	-	Consultant to the California Highway Department, active in boundary layer studies
North American Weather Consultants Santa Barbara Municipal Airport Goleta, California 93017	Letter	-	Use a statistical model rather than dispersion model. Model is being tested by the California Highway Department group
Andrew Ranzieri California Division of Highways Materials and Research Department 5900 Folsom Boulevard Sacramento, California 95800	Interview	Several papers, some data	

Table 1 (continued)

Name and Address	Contacted by	Response	Particular reason for contact
L. J. Shieh Scientific Center, IBM 2670 Hanover Street Palo Alto, California 94300	Letter	-	
Ralph C. Sklarew Systems, Science and Software P. O. Box 1620 LaJolla, California 92037	Letter	-	Active in developing photochemical models and use of mass conservation models
Systems Applications, Inc. 9418 Wilshire Boulevard Beverly Hills, California 90212	Letter	-	Interesting refinements done to a basic model
Systems Control, Inc. 260 Sheridan Avenue Palo Alto, California 94306	Letter	-	Interesting refinements done to a basic model
TRW Transportation and Environmental Operations Westgate Park 7600 Colshire Drive McLean, Virginia 22101	Letter	-	Have developed several models for EPA and have done sensitivity studies - to check on current research efforts
Dean Wilson Environmental Protection Agency 1200 Sixth Street Seattle, Washington 98101	Interview	Several papers	

Table 1 (continued)

Name and Address	Contacted by	Response	Particular reason for contact
John R. Zimmerman Division of Meteorology, EPA Research Triangle Park North Carolina 27711	Letter	Paper	

3.0 AIR QUALITY DISPERSION MODELS

Mathematical diffusion modeling for the purpose of air quality prediction is a complex and often controversial undertaking. The development and use of these models generally requires engineers, meteorologists, chemists, mathematicians, and others to adequately couple the many diverse components together. In addition, the development cost of large scale dispersion models is expensive and requires several man-years of effort.

The need to use mathematical models and the complexities and difficulties inherent in their development and use suggests the need to carefully scrutinize the situation to be modeled and to select the "best" model (tool) for that situation. It is doubtful that any one model will be acceptable for all applications, therefore a range of techniques should be available. Furthermore, each alternative must be user oriented so that the model calibration, applicability, scale, and limitations are carefully detailed.

In surveying the state-of-the-art in modeling there are two general approaches; either to examine each model as it is available or to examine the general aspects of basic model types. The former viewpoint tends to emphasize the commercially available models and provides a good background for selection of models that are already in use. In section 3.2 the individual models are examined in total.

Discussion of general aspects of model types, by its very nature tends to point favorably to some parts of a model but less favorably to other parts. Nevertheless the state-of-the-art is perhaps better assessed since no longer are total models pitted against each other, but rather, individual submodels are seen in juxtaposition. Section 3.1 is an evaluation of progress that has been made in modeling the individual components of dispersion models.

3.1 A General Discussion of Important Aspects of the Models

The essential components of an operational air quality prediction model for transportation systems are shown in Figure 2. As illustrated, the model includes five submodels: emission prediction, meteorological data preparation or calculation, the pollutant transport and dispersion model, the possible chemical reactions, and the topographic considerations. In the real world the different aspects of the problem are interrelated so that the assumptions used within each submodel limit the applicability of the whole model.

Air quality models attempt to simulate the action of the atmosphere in mixing, modifying, and transporting pollution from its source to any other point, usually designated as a "receptor." The general equation governing this interaction may be written:

$$\begin{aligned}\frac{\partial c_i}{\partial t} + u\,\frac{\partial c_i}{\partial x} + v\,\frac{\partial c_i}{\partial y} + w\,\frac{\partial c_i}{\partial z} &= \frac{\partial}{\partial x}\left(K_x\,\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\,\frac{\partial c_i}{\partial y}\right) \\ &\quad + \frac{\partial}{\partial z}\left(K_z\,\frac{\partial c_i}{\partial z}\right) + R_i\,(c_i, \cdots, c_n) + S_i \end{aligned} \tag{1}$$

There is an equation of this form for the concentration c_i of each of the $i = 1, \cdots, n$ pollutants considered. In this equation t is the time; x, y, z are cartesian coordinates; u, v, w are the components of the mean

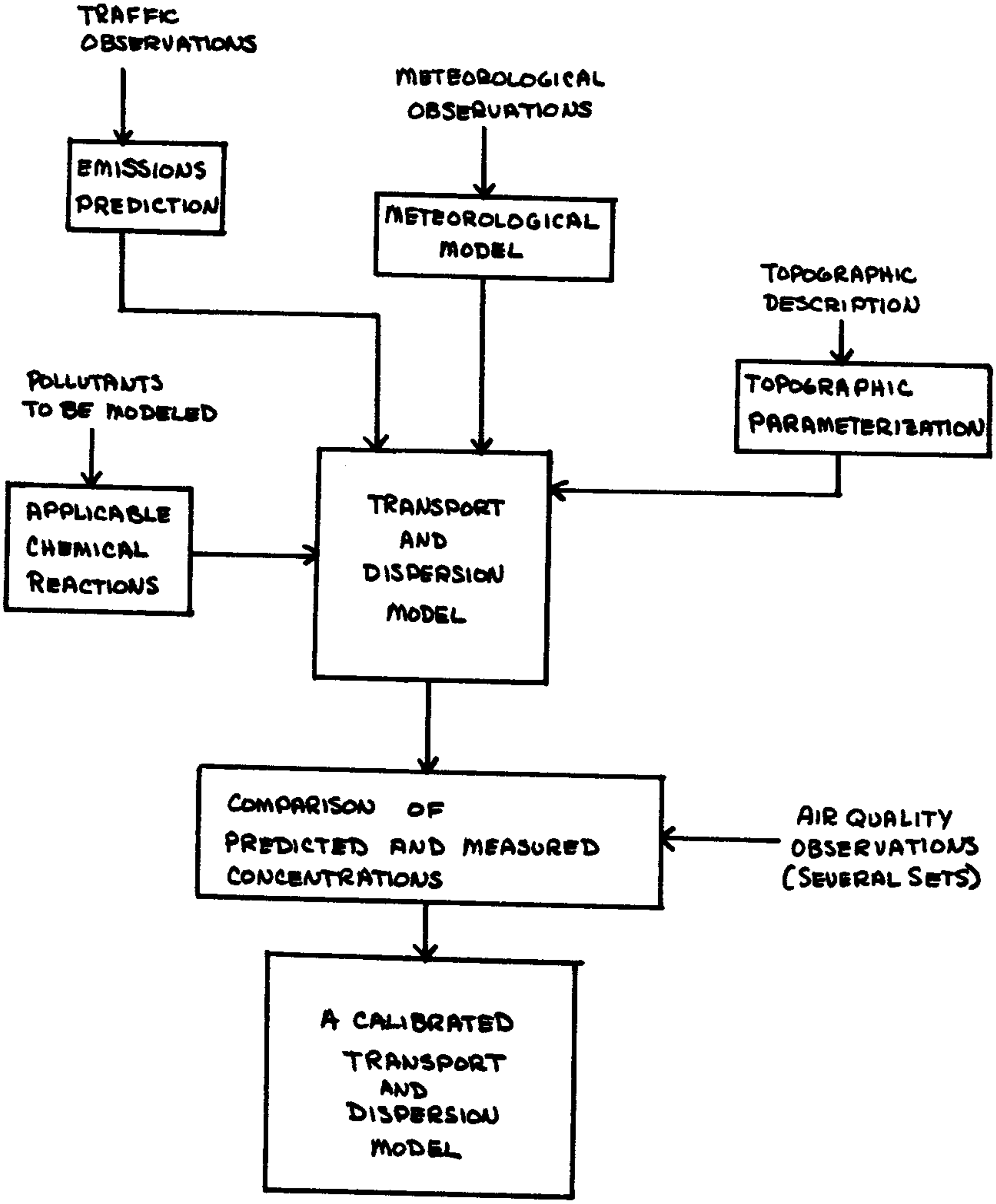


Figure 2: Essential components of an operational air quality prediction model

wind velocity in each of the coordinate directions respectively and are supplied from observations or may be derived from the equations of motion of the atmosphere; K_x, K_y, K_z are the eddy diffusion coefficients in each direction and are related to the temperature stratification (or stability) and to the wind shear, surface roughness, and convective heat flux; R_i is the rate of generation of the i-th pollutant by chemical reactions and may be a function of the concentrations of other pollutants thus coupling the equations for several pollutants (R_i is negative if the species is destroyed in the reaction); S_i is the source term including both emissions (positive S_i) and losses by deposition (negative S_i).

The first term in the dispersion equation shows the change of concentration with time. Models which assume this term is zero obtain "steady-state" solutions. The next three terms represent the advection or transport of the pollutants by the mean winds. The first three terms on the right hand side of the equation allow for the pollutant dispersion by turbulent eddies in the atmosphere. Molecular diffusion, where molecules move because of a concentration gradient, has been ignored because it is much smaller than the dispersion caused by the turbulent fluctuations in the mean winds. The last two terms account for the generation of the pollutant, the emission into the atmosphere, and the losses by chemical reaction or deposition. This equation and its associated boundary conditions form the basis for all the dispersion models discussed in this report. Figure 3 presents a schematic representation of this basic equation.

It is easy enough to write down the system of equations including the dispersion relations for each pollutant, the equations of motion for the atmosphere, and their associated boundary equations; it is much more of a problem to solve such equations subject to all the complicating and

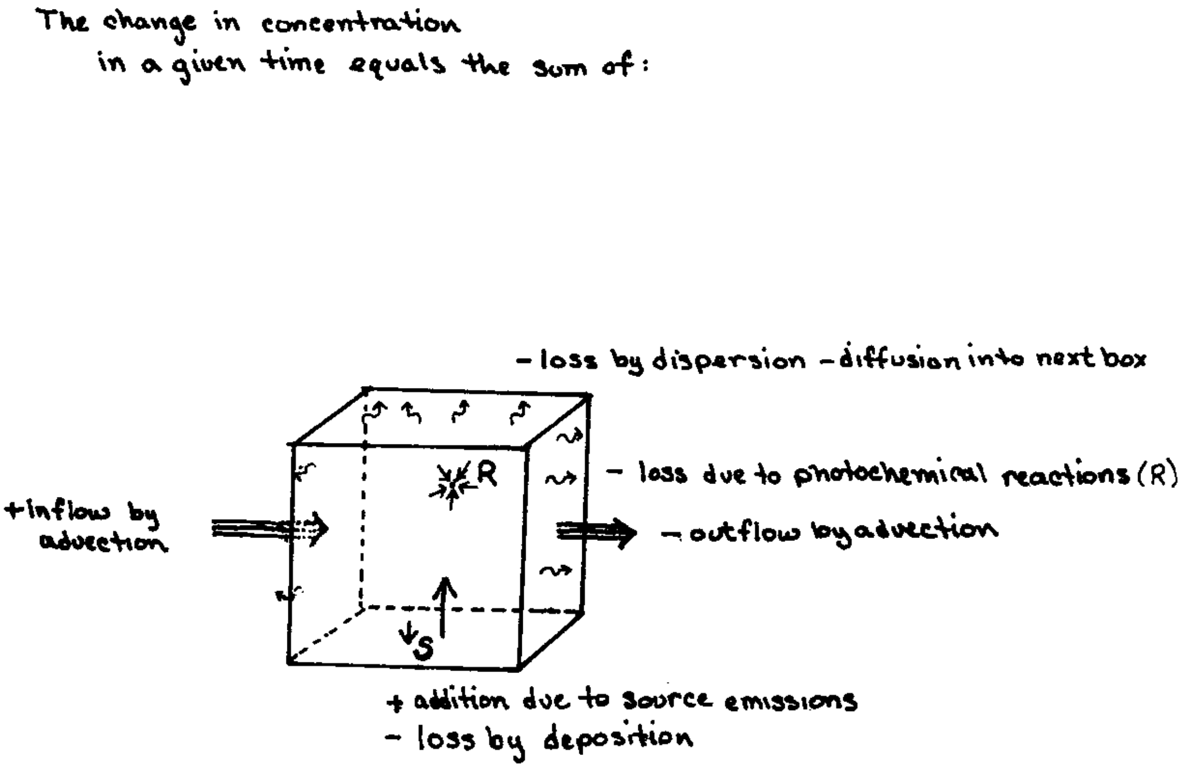


Figure 3: Representation of the basic advection-dispersion equation.

restricting conditions presented by variable sources, variable weather, the nature of the terrain, and the chemistry of the pollutants themselves. The situation is simplified by assuming that the pollutants do not influence the atmosphere. With such an assumption the dispersion equations are no longer coupled to equations governing atmospheric motions so that once u, v, w, K_x, K_y, K_z are specified the dispersion relation may be solved. The derivation of values for these six parameters and effects of the atmosphere on other aspects of pollutant dispersal are discussed in the next section as the "meteorology submodel." The treatment of the dispersion relation once the atmospheric parameters are specified are covered in the following section.

3.11 Meteorology

In theory one should consider the interlocking behavior of many meteorological variables: the wind in moving, diluting, and mixing pollutants; the temperature in influencing the rate of chemical reactions; the humidity in participating in the reactions both as ingredient and catalyst; the particulate content of the air as it influences and is in turn influenced by chemical reactions; sunlight as it modifies both the physical motions of the atmosphere and the chemical reactions that go on; and clouds and precipitation as they react with, and eventually remove pollution from the atmosphere. Of all of these, however, only the behavior of the wind is universally modeled. Serious attempts are being made to include chemical, especially photo-chemical reactions in some models but these are not yet satisfactory for operational use. Removal processes are not really modeled at all; either the pollutant is assumed to stay in the atmosphere forever once introduced, or an arbitrary rate of removal is assigned without regard to the meteorological variables that influence this removal.

ROLE OF THE WIND

Even when the problem is reduced to that of considering the action of the wind alone, it is difficult enough. Almost invariably the wind behavior is separated into two parts for modeling. Relatively large scale motions are described as "transporting" the pollution from source to receptor while relatively small scale motions are described as diffusing and mixing the pollutant as it is transported. Any visible plume from a smokestack illustrates the behavior that is being modeled. The plume is seen to stream off downwind under the influence of the larger scale motions, while it simultaneously spreads and becomes more dilute under the influence of the small scale motions.

In nature there is no sharp cut-off between the larger and smaller scales of air motion, nor can their roles in spreading pollution be entirely disentangled. In models the distinction is always made, either explicitly or implicitly, and consequently the mathematical treatment of the two scales is very different.

LARGE SCALE MOTIONS OR MEAN WINDS

The simplest models assume that the mean winds are constant in time and space, unchanging in either direction or speed. The appropriate values of the wind to put into the model come from observations of one sort or another. In a city of moderate size such as Seattle there may be five, ten, or more locations at which wind is measured consistently. Any one of these measurements, the average of all of them, or the reading of a single anemometer set up in a special location for a special test may be taken as the "mean" wind in such a simple model.

In more complicated and realistic models, mean winds can be modeled to vary from point to point. Such variation is known to occur both vertically and horizontally. In the vertical, wind speeds almost always increase with height. Models such as the Lawrence Livermore Laboratory simulation for the Bay Area, INTERCOMP, and General Research Corporation allow for vertical speed variation by using specified functions (in this case a "power law" of the form $u \propto z^n$). Wind direction changes with height are more difficult to specify and to fit into models. On the average in the northern hemisphere wind veers with height, i.e. shifts clockwise as height increases, but many variations are possible and only if the wind is measured or most carefully worked out from dynamic theory can realistic direction changes with height be incorporated into models.

Wind variability in the horizontal is both very common in nature and relatively difficult to incorporate into models in a realistic fashion. Nature does not, and it follows that models cannot, allow for entirely random differences in wind speed and direction from point to point. Complicated as the air flow may be it still must obey certain physical laws and these laws must not be violated, at least not seriously, in a mathematical model. The important principle is that of the conservation of mass both of the pollutant and of the air. To meet this requirement, models may incorporate more or less elaborate schemes.

Assuming that a self consistent, mass-conserving wind field for a metropolitan area is to be re-constructed from a few reported winds, the simplest method is to assume a constant, uniform wind field everywhere, the same assumption as described above. A more complicated but still simple method is to assume two-dimensional motion (that is, no vertical motion) derivable from a stream function. This type of flow has the property of not permitting convergence or divergence of mass. This approach is exemplified by the Connecticut model of Hilst.

A much more complicated resolution of the difficulty, and potentially more useful is the Lawrence Laboratory model for the San Francisco Bay area (MacCracken, et al.). This type of model is only feasible with one of the highest speed computers. This involves defining a wind field confined by the terrain below it and an inversion of variable height above it, making sure that it is consistent with whatever measured winds are available, allowing for only as much horizontal convergence of wind into or divergence out of any area as will be consistent with observed changes in inversion height, then using this wind field as an input to the diffusion model.

Whether simple or complicated, the procedures above illustrate the dilemma of the meteorological modeler and require a word of caution. This dilemma is very similar to that always confronting the weather forecaster and is sorely felt within the meteorological community but little appreciated outside of it. First, there are never enough observations (in this case wind observations) to completely specify the state of the atmosphere. Second, if there were enough such observations there would be no feasible way of incorporating all the pertinent information into a computer model. Third, using the amount of information that is available permits finding a solution (in this case a set of winds for a metropolitan region) that conforms to existing observations and violates no physical laws but which may not correspond in detail with the actual wind field at points where no observations exist.

The user of air quality prediction models would, of course, like to have accurate, specific predictions for every point in the area of concern, but it must be realized that this is impossible at present and unlikely for the future. Even in concept, if predictions were to be requested for each square block, for example, and for each ten minute period of the day it would be impossible for any model to furnish this information unless meteorological information and source contributions were known with at least as much detail. This is not apt to become true and even if it were, evaluating and analyzing the data and developing a model of sufficient refinement to use the information would be a formidable task involving large amounts of computer time and storage which would make it uneconomical in most cases.

SMALL SCALE, TURBULENT, DIFFUSIVE AIR MOTIONS

Regardless of how the large scale winds are handled there are other small scale motions, turbulent eddies of such limited size and lifetime that they cannot be known in detail. Their role in diffusing pollution is handled in several ways.

The method that has become most common in the last 10 years is that due to Pasquill and modified by others, notably Gifford. It is well described in Meteorology and Atomic Energy, 1968, edited by Slade. This method is usually applied to point sources such as stacks but with appropriate and simple modifications it is adaptable to line sources such as highways, to puffs or clouds of pollutants as from an explosion, or to "area" sources, that is, small sources more or less uniformly distributed over an area.

Pasquill's method is based on empirical data that have shown how the spread of a plume is related to the distance from the source and to the meteorological conditions which control turbulent eddy mixing. Meteorological effects are put into one of six categories: A (most unstable, most active mixing), B, C, D (neutral stability), E, F (most stable, least mixing). The original categorization was on the basis of wind speed, cloudiness, and intensity of sunshine. Later models have retained the same categories but have used observation of wind gustiness or vertical temperature gradients (lapse rates) to select the proper category for a given diffusion case.

Having chosen the proper meteorological category, one enters tables or charts to find the expected spread of the pollution cloud at various downwind distances from the source. The spread is given in terms of the standard deviation of the distance the pollution has spread from the centerline of the puff or plume. This together with the assumption of a Gaussian or "normal" distribution and the conservation of mass of the pollutant, then allows an estimate of concentration at any point downwind from the source.

Another common method of accounting for the role of small wind eddies is to use eddy diffusivity or "K" theory in the manner of equation (1). This assumes that turbulent eddies act in such a way as to bring about a flux of pollutant in a down-gradient direction. That is, there will be a movement of pollutant from region of higher concentration to regions of lower concentration and this flow or flux (mass per unit area per unit time) is proportional to the eddy diffusivity and to the change of concentration per unit distance across the area. This is also called Fickian diffusion and is analogous to fluxes of heat (heat conduction), mass and momentum by molecular motions in a non-turbulent fluid.

Although at first glance K theory would appear quite different from Pasquill's and similar approaches, there is really a great deal of similarity between them. In fact where they can both be applied to the same problem there is a simple relationship between σ^2, the variance or squared standard deviation and K

$$\frac{d\sigma^2}{dt} = 2K \tag{2}$$

the rate of change of σ^2 equals 2K. The meteorological problem ~~then~~ reduces to that of choosing the best K for a given set of variables.

The advantage of K theory over the Pasquill method is its much greater versatility. However, it requires much greater computing time and involves a greater chance of computational errors.

K theory, partly because of a basic imperfection in the theory and partly because of computational difficulties, is apt to give poor results near the sources of pollution. It can be used, however, for long-term problems with changing winds, changing stabilities, and vertical and horizontal differences of meteorological variables. In other words, it can take into account many more types of cases and more complicated cases than Pasquill's or similar models.

Table 2 compares the ways different models handle large and small scale motions.

3.12 Dispersion Models

In the literature, the various air quality models are generally differentiated by the technique used for solving the pollutant dispersion relation, equation (1). The general types of solutions determine the meteorological input that can be handled and the applicable geographical scales. Assumptions inherent in deriving the solutions limit the range of cases that can be handled. Understanding the assumptions involved in the derivations and the limitations of each model are imperative.

Table 2. Meteorological parameterizations.

Model	Large Scale Motions	Small Scale Motions
Aerovironment	horizontal velocity a function of time only	$K_h = (\lambda a_z)^2 t$ $K_z = a_z^2 t$ a_z is a dispersion speed which is a function of surface roughness, wind speed, and heat flux
Argonne National Laboratory	stability class mean horizontal wind	σ_y, σ_z by Pasquill-Gifford curves
California	mean wind stability class	σ_y, σ_z of Pasquill-Gifford but extended to small downwind distances
Center for the Environment and Man	equations of motion for the atmosphere are solved the energy equation, temperature distribution is calculated	K_z is a function of the Richardson number and height
Chen	constant mean wind	$\sigma_z = \frac{1}{\sqrt{2}} C_z \; X^{(2-n)/2}$
Danard	mean wind measured at 10 meters, wind speed, direction and temperature advection above	K_x, K_z are functions of wind speed, height, roughness, distance from roadway; wind speed varies with height
Environmental Protection Agency	stability wind rose	σ_y, σ_z from Pasquill-Gifford curves
ESL, Inc.	mean wind	σ_y, σ_z from measured deviations in lateral and vertical wind directions
General Research Corporation	wind speed and direction from trajectories	K_z trapezoidal dependence with height for urban model, a function of aerodynamic drag for roadways

Table 2 (continued)

Model	Large Scale Motions	Small Scale Motions
Gifford and Hanna	stability, mean wind	M is related to $\sigma_z = aX^b$ where a and b are determined from Pasquill-Gifford curves
Hilst	measured wind field adjusted to be mass consistent	σ_y, σ_z determined from Pasqukll-Gifford curves
INTERCOMP	a modified velocity potential is used to allow the horizontal velocity to vary with height	K_x, K_y, K_z are input and may be varied to calibrate the model
Lamb and Neiburger	trajectories are determined from streamline-isotach analyses of available data	K_h, K_z are specified constants
Lawrence Livermore Laboratory	the observed wind field is used to construct a wind field that conserves mass where topography and inversion heights may vary with space and time	K_h is a function of the eddy dissipation rate and a length parameter K_z is a function of wind speed
Mathematical Sciences	mean wind, stability	σ_y, σ_z from Pasquill-Gifford curves
Shieh	mean wind direction and speed, inversion heights both as functions of time	σ_y, σ_z given as functions of time
Sklarew, S^3	streamline-isotach charts of Lamb were used	K_h, K_z constants
Stanford Research Institute	stability wind rose	σ_y, σ_z from Pasquill-Gifford curves
The Research Corporation	stability wind rose	σ_y, σ_z from Pasquill-Gifford curves
Turner	stability wind rose	σ_y, σ_z from Pasquill-Gifford curves

The problem of fluid flow including diffusion can be described in terms of a reference grid fixed with respect to the ground (Eulerian) or in terms of the history (specifically the location and pollution concentration) of a set of identifiable air parcels (Lagrangian). In a free-wheeling discussion of a diffusion problem one may jump back and forth between these two concepts, but if the problem is to be treated mathematically one or the other or a specified combination of the two must be adapted and adhered to.

For modeling the more common is the Eulerian frame in which sources are located, winds are described, and concentrations computed or measured at specific points in a fixed grid. Equation (1) has been written with this formulation in mind.

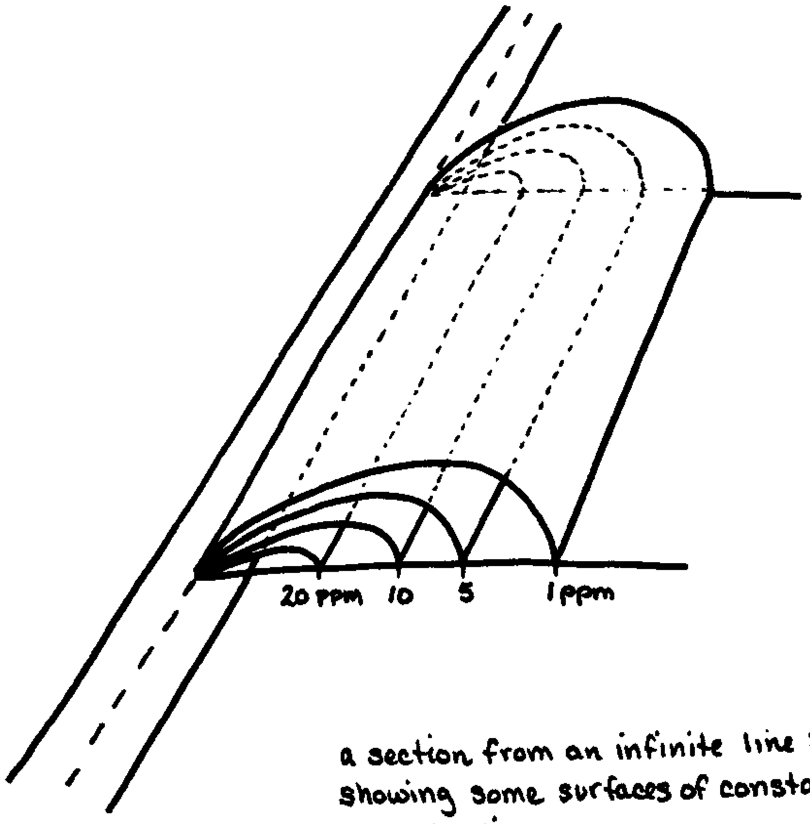
The diffusive part of the pollution problem, however, is more naturally formulated in terms of a moving air parcel, that is in a Lagrangian frame, and for that reason a few models attempt to use this method. Two difficulties arise, however; sources are more easily described in a fixed frame, and continuity (i.e., conservation) of mass is much harder to express in Lagrangian coordinates. For these reasons no model uses a pure Lagrangian system, but some, what may be called moving-cell models, incorporate a quasi-Lagrangian set of parcels in a basically Eulerian frame.

GAUSSIAN PLUME MODELS

The Gaussian plume model illustrated in Figure 4 is basically an analytical solution for a simplified version of equation (1).

$$u \frac{\partial c}{\partial x} = K_y \frac{\partial^2 c}{\partial y^2} + K_z \frac{\partial^2 c}{\partial z^2} \qquad (3)$$

Obviously, this equation will have a steady state solution. It is valid in a Eulerian system where turbulent diffusion in the x direction, parallel



a section from an infinite line source
showing some surfaces of constant
concentration

Figure 4. Gaussian plume model

to the mean wind u, is assumed to be much less important than the advection in that direction. The solution to (3) must also satisfy the continuity equation

$$\int_A ucdA = Q \qquad (4)$$

or the rate of transfer of matter across the plane perpendicular to the wind direction must equal the source strength Q. Boundary conditions must also be specified. The most common conditions are that the concentration approaches zero far from the source and it approaches infinity at the source. The formal solution to this set of conditions is

$$c = \frac{Q}{4\pi x\ (K_y K_z)^{1/2}} \exp\left[- \frac{uy^2}{4K_y x} - \frac{uz^2}{4K_z x}\right] \qquad (5)$$

This solution is not in the form usually used, but the substitutions $\sigma_y(x)^2 = 2K_y \frac{x}{u}$ and $\sigma_z(x)^2 = 2K_z \frac{x}{u}$ (which both reduce to equation (2)) transform (4) the more familiar form

$$c = \frac{Q}{2\pi u\ \sigma_y(x)\ \sigma_z(x)} \exp\left[- \frac{y^2}{2\sigma_y{}^2(x)} - \frac{z^2}{2\sigma_z{}^2(x)}\right] \qquad (6)$$

Note that the form for the solution gives a normal or Gaussian distribution of the pollutant in both the horizontal and vertical directions. The standard deviation of each curve is just σ_y or σ_z.

Modifications of this basic model are diverse and interesting to consider because they extend the applicability of the solutions. Equation (6) assumes a ground level source and a receptor at height z. Allowance can be made for a source with height h. The interaction of the pollutant with the ground generally treated as either total reflection or total absorption at the ground surface. One model (ESL, Inc.) defines a variable P as a percentage of reflection. A decay term is sometimes added to allow for very simple loss mechanisms. The decay coefficient λ may be empirically derived or may be based on some simple chemical reaction rate. An equation incorporating all of these refinements may be written:

$$c = \frac{Q}{2\pi u\sigma_y(x)\sigma_z(x)} \exp\left(-\frac{\lambda x}{u}\right) \exp\left(\frac{-y^2}{2\sigma_y(x)^2}\right) \cdot \left[\exp\left(-\frac{(z-h)^2}{2\sigma_z(x)^2}\right) + P \exp\left(-\frac{(z+h)^2}{2\sigma_z(x)^2}\right) \right] \tag{7}$$

The concept of a mixing cell or a virtual source has been used to allow an initial spread σ_{yo} or σ_{zo} to the plume. Mixing cells have been of particular value in highway models since the motion of motor vehicles tends to mix the air immediately above the traffic lanes more completely. Concentrations calculated within this region are not Gaussian.

Perhaps the most important refinement to the basic Gaussian plume models is the extention to line and area sources. The line source equations may be obtained by integrating either equation (6) or (7) (without the decay term) over many point sources lying along a line in the y direction. This equation

$$c = \frac{Q}{\sigma_z(x)u} \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z(x)^2}\right) + P \exp\left(-\frac{(z+h)^2}{2\sigma_z(x)^2}\right)\right] \tag{8}$$

can be extended to handle all wind directions to within 10 to 12 degrees of being parallel by taking the x component of the mean wind; that is, u in equation (8) is replaced by U sin θ, see Figure 5. The case for $\theta < 12°$ must be handled separately, usually as a modification of the point source solution. The Gaussian plume solutions are not valid for cases of zero winds and low-level inversions. Separate approximations may be devised to take care of these cases.

The Gaussian plume models are widely used. The advantages of such closed-form solutions are their simplicity and ease of application and ready modification to graphical or tabular form. The data required as input is readily available and numerous studies have been carried out on the sensitivity of these equations to different input values. These advantages must be weighed against the disadvantages of the simplifications required to get the solutions. Sources are assumed to be emitting continuously so that special approximations must be invoked in order to look at the changes of concentrations with traffic cycle. The meteorological variables are assumed to be uniform in time and space. For short times and distances this is not a bad assumption, but this may prove troublesome in some cases. Reactive pollutants cannot be considered. The solution is not valid for light winds. The effects of topography are difficult to incorporate.

Table 3 summarizes the refinements of the basic Gaussian plume model used by specific modelers.

GAUSSIAN PUFF MODELS

Gaussian puff models have been developed to improve on some of the disadvantages of the plume models. Both steady-state and time dependent solutions have been developed. Transformation of equation (1) to the Lagrangian system of coordinates makes the equations more tractable and closed form solutions are available. The reaction and source terms are

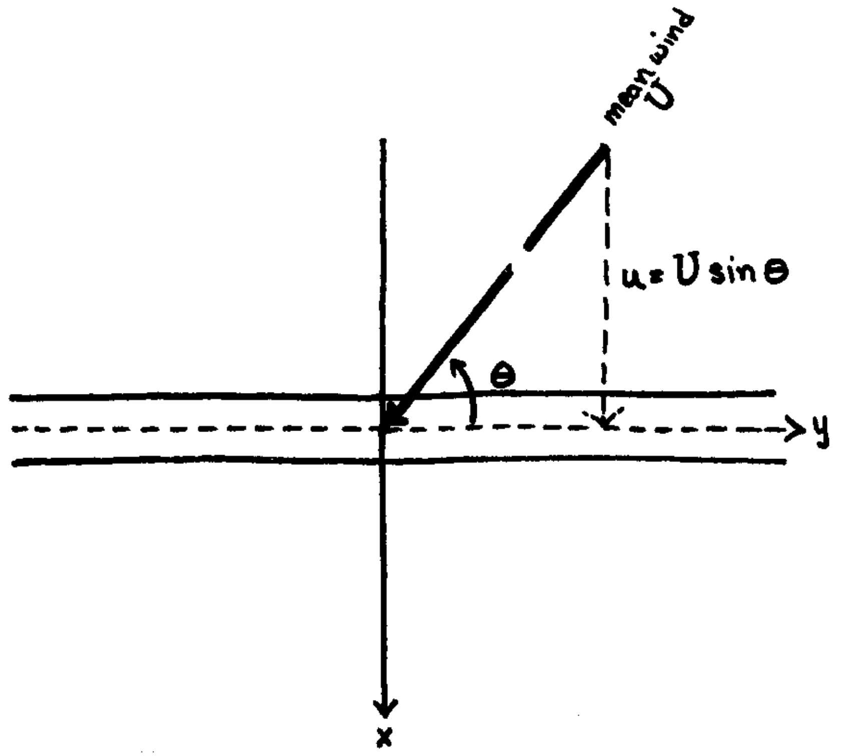


Figure 5. Cross wind component of the mean wind

Table 3. Refinements of the basic Gaussian plume model.

model	modifications to basic equation	additional features
California	formulas for depressed receptors and depressed sources	use of mixing cell over highway
Chen	point source moving parallel to the wind	reflection of plume at sidewalls of depressed highway
Environmental Protection Agency	cut sections modeled as an area source	
ESL, Inc.	percentage of reflection at ground allowed	removal by ground adsorption modeled as a 'tilted' plume
Gifford-Hanna	area source modeled by simplified formula	dry deposition and precipitation scavenging
Hilst	downwind distance x changed to receptor coordinate minus source coordinate	decay term
Shieh	area source integrated numerically	
Stanford Research Institute	infinite line source formula used	
The Research Corporation	finite line source formula of Turner modified for skewed winds	
Turner	virtual sources	formulas for different averaging times

neglected. The conservation equation similar to equation (4) is necessary the boundary condition c (x-ut, y, z, t) = δ (x-ut, y, z, t) where δ is the Dirac delta function is imposed. The solution to this set of conditions represents the concentration due to an instantaneous release at t=0, x=0, y=0, z=0 and is

$$c(x,y,z,t) = \frac{Q(t)}{(2\pi)^{3/2}\sigma_x(t)\sigma_y(t)\sigma_z(t)} \exp\left[-\frac{(x-ut)^2}{2\sigma_x(t)^2} - \frac{y^2}{2\sigma_y(t)^2} - \frac{z^2}{2\sigma_z(t)^2}\right] \quad (9)$$

The x direction has been defined as parallel to the mean wind. Note that the concentration is time dependent due essentially to the changes in σ and Q along the trajectory of the puff. Also, the term outside the exponential is no longer proportional to 1/u so that the solution remains valid for light wind conditions.

As in the case of the plume models refinements for elevated sources and receptors are possible. A similar decay term may also be used. Line source formulas have been developed for the general case of highways at any angle Θ to the mean wind. When the angles are small the same formula applies but the line must be broken into shorter segments.and contributions from each segment must be added.

These models follow the history of a puff of pollutant as it is blown downwind and disperses in a Gaussian manner, see Figure 6. In order to correctly predict concentrations at a receptor downwind the trajectories of the air flow must be accurately known and the puff following a trajectory must pass over the receptor. Both the determination (or storage) of the trajectory pattern and the number of puffs that must be followed in order to get a fair representation of the concentrations over the area studied require the use of computers.

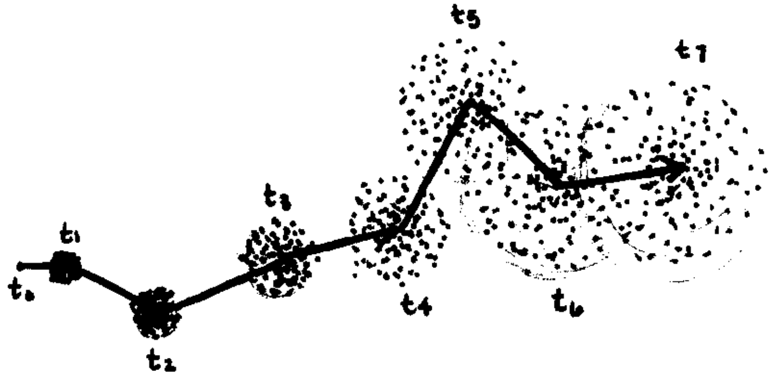


Figure 6. Gaussian puff in a variable wind field

Topography, as in the Guassian plume models, is difficult to incorporate. Background contributions to the pollutant load are better incorporated since they can be allowed to vary in time. The model of Lamb and Neiburger is really of a type somewhere between the Gaussian puff model and the mass conservation model. Their model incorporates the sources in the source term rather than in the auxiliary conservation equation and obtains analytical solutions allowing for initial background contributions and some simple chemical reactions (first order).

The computational requirements of time and storage space seem to be the major disadvantages to this approach.

MASS CONSERVATION MODELS

This type of model has been developed only recently and allows the most flexibility in handling complicated problems. Mass conservation model is perhaps a misnomer since the plume and puff formulations must also conserve mass. The primary difference between the plume/puff approach and the one described in this section is that the differential equation (1) is solved numerically rather than analytically. Simplifications necessary to get closed form solutions (like K's independent of position, R_i zero or linearly proportional to c_i) need not be imposed. Approximations are made primarily to reduce computer storage or running time. As in most finite difference schemes the choice of space or time grid sizes may present problems. Some models encounter difficulties with "artificial diffusion" where the pollutant in one box diffuses some small amount into the neighboring boxes where it is assumed to be well mixed. This leads to extra diffusion into boxes farther away in the next time step, see Figure 7. The advection terms give rise to this effect in the horizontal.

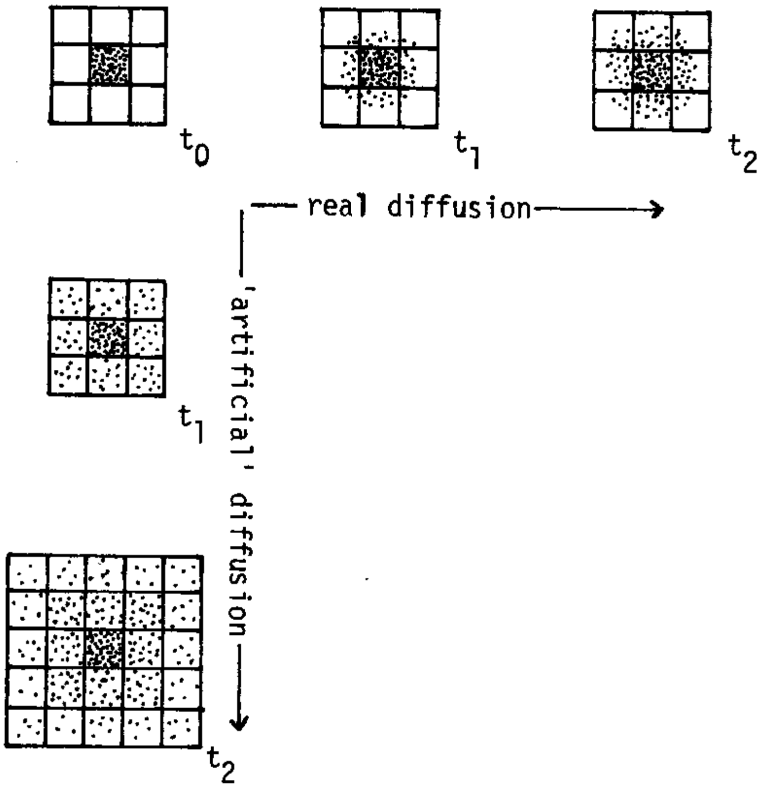


Figure 7. Artificial diffusion

In spite of these disadvantages, these models are potentially improvements over the Gaussian plume and puff models. The mass conservation models allow the treatment of chemical reactions of higher order, the detailed specification of the initial background concentrations, K's and winds variable in the horizontal and especially in the vertical, and they can include topographic effects as expressed in the wind field and the lower boundary conditions. The input requires values for the winds at grid size intervals while observations are usually much more sparse. These models have been applied to both regional (urban) and local (highway) problems.

There are four principal types of mass conservation models depending on terms in equation (1) that have been retained. Boundary and initial conditions are required in each type and will influence the final concentrations calculated.

The numerical solution of equation (1) with the modification $K_x=K_y=K_h$ in a Eulerian frame of reference has been attempted by several groups (early model of Eschenroeder and Martinez, INTERCOMP, and others). It can be applied to urban-wide problems as well as highways and is more physically realistic then most approaches. Chemical reactions can be handled although not as well as in a Lagrangian frame of reference and topography is readily included by setting the K's to zero at the lower boundary. Artificial diffusion is a definite problem in these models and computer requirements are large.

Multiple-box models use a Eulerian grid of boxes through which cells of pollutants move. The Lawrence Livermore Laboratory and others have developed this approach. In the Lagrangian frame the basic equation used is:

$$\frac{\partial c_i}{\partial t} = K_h \left[\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2}\right] + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_i}{\partial z}\right) + R_i + S_i \qquad (10)$$

The height of the grid boxes is a function of varying inversion heights and the size of the pollutant cells is allowed to vary. The partial differential equations can be reduced to a series of ordinary differential equations. The handling of topography by varying the heights of the bottom of the boxes and use of a pollutant lifetime to approximate the air chemistry make this model fairly versatile. Artificial diffusion can again be a problem although the LLL model seems to have it under control. Computer times are modest.

The particle-in-cell model developed mainly by Sklarew examines the movement of particles that represent the pollutant mass. The velocities of these particles is the mean velocity, plus a turbulent velocity which approximates the K-theory diffusion. The basic equation used is of the form

$$\frac{\partial c_i}{\partial t} + \frac{\partial}{\partial x}(u'c_i) + \frac{\partial}{\partial y}(v'c_i) + \frac{\partial}{\partial z}(w'c_i) = R_i + S_i \qquad (11)$$

This approach avoids the problem of artificial diffusion and produces a concentration pattern for the area under study. The large computer storage requirements for following all of these particles is a definite problem. Air chemistry is not handled very well.

The moving-cell model developed mainly by Eschenroeder and Martinez is well suited to handling air chemistry reactions. Two models are available, one with no horizontal diffusion:

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial c_i}{\partial z}\right) + R_i + S_i \qquad (12)$$

the other with an analytical solution for horizontal diffusion:

$$\frac{\partial c_i}{\partial t} = K_h(z) \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial}{\partial z} (K_z(z) \frac{\partial c_i}{\partial z}) + R_i + S_i \qquad (13)$$

where these equations are in the coordinate system moving with the cell. Cells stacked in the vertical and horizontal are used. Since computer time requirements are modest, more time is available for chemical rate calculations.

OTHER MODELS

Aeronautical Research Associates of Princeton and INTERCOMP have developed or are in the process of developing finite difference solutions to the complete Navier-Stokes equations. These equations can model difficult aerodynamic problems like split-flow and flow around obstacles and bridges. These approaches require large amounts of computer time.

North American Weather Consultants uses a statistical model to predict pollution concentrations. Details of this process were not available for this study.

3.13 Emissions

Although the primary emissions of motor vehicles are carbon dioxide, water vapor and heated air, these are contaminated by carbon monoxide (CO), hydrocarbons (HC), nitrogen oxides (NO_x), and particulates. The problem of estimating the source strengths for any one of these pollutants is complicated by the variability of emissions due to different kinds of motor vehicles, the fact that they are moving on the highway (sometimes at different speeds), that for a particular vehicle the emission is dependent on many factors peculiar to that engine (e.g., engine age, compression ratio, air-fuel ratio, timing, misfiring, kind of fuel used), engine speed, mode of driving (cold start or hot start), load (like weight carried or going up a hill), and meteorological factors (like intake temperature and relative humidity), altitude, and the working condition of air pollution control devices if any.

Obviously, each and every car, truck, or bus could have a different function relating these details to the actual emissions. Since in general the kind of functional relationship there is between emissions and all these factors is not known precisely, measurements of the effects of some and assumptions about the others are necessary.

The total emissions, usually given in grams per second per meter of roadway, equals the traffic volume (the number of vehicles per hour) for a stretch of road of a particular length (in miles), multiplied by an emissions factor in units of grams per vehicle mile, times conversion factors:

$$\text{Total Emissions} = \text{traffic volume} \times \text{emissions factor} \times \frac{\text{miles}}{\text{meter}} \times \frac{\text{hours}}{\text{second}} \quad (14)$$

Several approximations for the traffic volume are used in air quality models. Generally annual or daily averaged values for the traffic are the data supplied and then a function based on measured hourly volumes is used to convert these values to hourly averages. The model developed by the Research Corporation (TRC) includes traffic speeds related to the traffic flow and the time of day. A maximum capacity is specified and the model does not allow additional cars to enter the segment when there is a traffic jam.

The emissions factor is the most complex feature of the emissions calculation, since it includes many characteristics of the different vehicles using the highways. Many factors are assumed to have small effects.

These first assumptions are generally a) meteorology has no effect on emissions, b) the terrain is flat, c) the general engine characteristics can be incorporated into or related to things like type of vehicle, age, mode of driving, and a deterioration factor, d) control devices are related to the model year of the vehicle which can be incorporated in the age, e) control devices if they are supposed to be working are working, f) the load being carried (no longer related to topography) can be incorporated into the type of vehicle. With these simplifications the emissions factor becomes a function of the pollutant, the type of vehicle, speed, driving mode, age, and the deterioration factor.

The dependence of the emissions on the age of the vehicle is clear since legislation has specified maximum permissible amounts of certain pollutants with respect to vehicle model year. If the proportion of 1970 cars in the total traffic volume is known, then their contribution to the total emissions is known. By summing over the model years the emissions factor may be found

$$e_{np} = \sum_{i=n-12}^{n+1} c_i \times d_i \times m_i \times S_i \qquad (15)$$

where e_{np} = emission factor in grams per vehicle mile for calendar year n and pollutant p.

c_i = emission rate for the i^{th} model year (from standards)

d_i = deterioration factor

m_i = annual travel of the i^{th} model year during calendar year n

S_i = speed adjustment factor.

The next most important factor in determining the emissions factor is the vehicle speed. One model was developed by SRI,

$$e = a \times S^{-b} \tag{16}$$

where S is the speed in miles per hour and a and b depend on the year and vehicle mix (only applicable to CO). All other models that include such an effect base their functions on work by Rose, et al., whose work is really only applicable to pre-1968 model cars. The emissions model suggested for use by the EPA, as well as models developed by Argonne National Laboratory, the California Highway department, and Lamb and Neiburger use the functions derived by Rose for CO and HC. Emissions are assumed to be independent of speed for later model vehicles. Reliable curves for NO_x have not yet been derived. Clearly, there is much research needed in this area at the present time.

The Argonne, EPA, and California models divide the vehicles into weight classes. Argonne and EPA specify five categories 1) passenger cars, 2) light duty trucks, 3) trucks from 6000 to 10,000 lb GVW, 4) trucks from 10,000 to 19,000 lb GVW, and 5) trucks greater than 10,000 lb. The California models consider only two classes; light duty vehicles (classes 1 and 2 above) and heavy duty vehicles (classes 3, 4, 5). Emissions factors are calculated for each type of vehicle for each model year for appropriate speeds and these factors are summed after being weighted by the fraction of the total vehicle miles that were driven by that model of the particular vehicle class.

A deterioration factor is sometimes included in the emissions factor to relate the miles driven to the less efficient functioning of the engine or the control devices. It is not clear how reliable these factors are.

Finally, it has been recognized that there are different modes of driving that can give rise to different emission rates. The EPA distinguishes between urban and rural, the primary difference being average speed. The California model makes the distinction between freeway driving and city street driving. They use one set of road tests for the freeway model and another set of tests for the street model. The Argonne model distinguishes between cold start driving (within the first two or three minutes of starting up the car) and hot driving. There is some evidence to show that emissions are largest in the first few minutes since some control devices take some time to reach peak efficiency.

Table 4 summarizes the models with respect to the emissions submodels.

3.14 Air Chemistry

Air chemistry models tend to concentrate primarily on the chemical reactions ignoring transport, diffusion, and winds; or they start out as dispersion models and a source term is included to allow for changes due to chemical reactions. The first approach can handle complex reaction systems with many species but must assume the concentrations to be fixed and known for some period, while in fact the reactants are rapidly dispersing thereby decreasing the likelihood of the reactions. The second approach is limited in that many reactions are of a higher order, that is the rate of formation is proportional to the concentration of some species squared or cubed. Only reactions of first order are easily handled by these methods.

Table 4. Emissions submodels

model	standards used	speed approximation	deterioration factor	pollutants	types of vehicles	driving modes
AeroVironment	CAL	Rose-modified	yes	CO	LDV/HDU	freeway/city street
Argonne	EPA	Rose	yes	CO	5 classes	hot/cold
California	CAL-EPA	Rose-modified	yes	CO, HC	LDV/HDV	freeway/city street
CEM	emissions from model of Roth, et al.			CO		
Chen	no emissions submodel discussed					
Danard	constant value	no	no	CO	one	one
EPA	EPA	Rose	yes	CO, HC	5 classes	urban/rural
ESL, Inc.	not discussed but probably CAL					
GRC	-	probably Rose	no	CO, O_3, NO, NO_2	one	one
Gifford-Hanna	source inventory					
INTERCOMP	constant value used			CO		
Lamb-Neiburger	-	Rose	no	CO	all same	only one
LLL	emissions inventory, daily traffic cycle			CO		
Math. Sci. NE	EPA	Rose	yes	CO	5 classes	urban/rural
Shieh	source inventory			SO_2		
Sklarew	emissions inventory, some traffic pattern data			CO		
Stanford Research Institute	α, β	$\alpha S^{-\beta}$	no	CO	all same	only one
TRC	EPA	Rose	yes	CO	5 classes	urban/rural
Turner	Not specified					

Since the dispersion equation itself is complicated, including non-linear reaction terms makes even numerical solutions difficult.

The models which appear promising in solving some of these difficulties are those of ESL, General Research Corporation, and Hecht and Seinfield. The ESL model uses a Gaussian plume dispersion model alternately with chemical reaction mechanisms so that for a short enough time step the assumption is that the process can be treated as alternating pure diffusion and pure chemical reaction. Eschenroeder and Martinez's model and the Hecht-Seinfield model solve the diffusion and reactions simultaneously but the chemical reaction rates have been lumped into several parameters involving the main pollutant components. In this way several reactions can be reduced to one net reaction with a modified rate constant to account for the in-between steps. Table 5 summarizes the reactions included in these three mechanisms. By far, the majority of the models to be discussed ignore air chemistry and thus restrict themselves to such gases as CO and SO_2 which do not react rapidly. Recent studies indicate that these gases often called inert may in fact react fairly rapidly. In the presence of water vapor reactions involving SO_2 may proceed fast enough that they become significant, especially where SO_2 is absorbed into water droplets forming sulfuric acid on a time scale of less than an hour.

The area of photochemical modeling is one to watch closely. There should be some acceptable models available in the next one to two years. EPA is currently trying to validate such models to include in their UNAMAP setup.

Table 5. Generalized mechanisms for photochemical smog.

		ESL	E&M	H&S
main inorganic cycle	$h\nu + NO_2 \rightarrow NO + O$	✓	✓	✓
	$O\ (+ O_2) + M \rightarrow O_3 + M$	✓	✓	✓
	$O_3 + NO \rightarrow NO_2\ (+ O_2)$	✓	✓	✓
hydrocarbon attack; chain initiation	$O + HC \rightarrow a\ RO_2\cdot$	✓	✓	✓
	$OH\cdot + HC \rightarrow b\ RO_2\cdot + c\ RCHO$		✓	c=0 ✓
	$O_3 + HC \rightarrow d\ RO_2\cdot + e\ RCHO$	✓	✓	e=0 ✓
source for HO_2	$OH\cdot + CO\ (+ O_2) \rightarrow CO_2 + HO_2\cdot$			✓
rapid NO oxidation	$NO + RO_2\cdot \rightarrow NO_2 + fOH\cdot$		✓	✓
	$NO + HO_2\cdot \rightarrow NO_2 + OH\cdot$			✓
products formation	$RO_2\cdot + NO_2 \rightarrow$ Products (e.g. PAN)		✓	✓
	$HO_2\cdot + NO_2 \rightarrow HONO + O_2$			✓
	$NO_2 + OH\cdot\ (+ M) \rightarrow HNO_3\ (+ M)$ α		✓	
	$NO_2 + O_3\ (+ NO_2 + H_2O) \rightarrow 2HNO_3\ (+ O_2)$ β			✓
	$NO + OH\cdot\ (+ M) \rightarrow HONO\ (+ M)$ α		✓	
alternate paths for HONO	$NO + NO_2\ (+ H_2O) \rightarrow 2\ HONO$ γ		✓	✓
	$h\nu + HONO \rightarrow OH\cdot + NO$		✓	✓

•	represents a free radical (unpaired electron)
$h\nu$	represents energy from sunlight
M	a third body (like N_2) which acts as a catalyst
N_2	molecular nitrogen
O_2	molecular oxygen
O	atomic oxygen
O_3	ozone
NO	nitric oxide
NO_2	nitrogen dioxide
CO	carbon monoxide
CO_2	carbon dioxide
$OH\cdot$	hydroxyl radical
H_2O	water vapor
$HO_2\cdot$	hydrogen dioxide free radical
$RO_2\cdot$	a generalized free radical where R may represent any HC chain
HC	a hydrocarbon (usually 'averaged,' could be trans-2-butene, propylene, ethylene, etc.)
PAN	peroxyacetyl nitrate
HNO_3	nitric acid
HONO	nitrous acid
a,b,c,d,e	chain branching factors
f	a fractional yield factor
α	rate constant lumps third body concentration
β	combination of three reactions
γ	water vapor lumped into rate coefficient

3.15 Topography

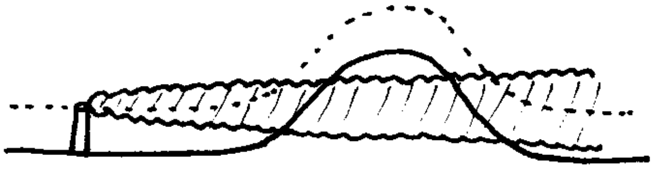
Topography in the context used here includes any terrain which is not flat including cut sections of highways, buildings, forests, mountains, land-sea effects, etc. Gaussian plume and puff type models can handle only the simplest effects and those only approximately. Cut and elevated sections and hills can only be treated as if the source or receptor were elevated. The air flow patterns are either horizontal or are parallel to the surface (see Figure 8). The AeroVironment model includes an attempt to handle some topography in their use of surface roughness. This parameterization acknowledges that trees and buildings influence the velocity field and attempts to take this into account.

Conservation of mass models are more suited to include topographic effects, but most must derive the velocity field from a few scattered observations. They cannot predict when split flow might occur (see Figure 9) and they cannot yet handle the effects of variable winds aloft or land-sea breeze effects.

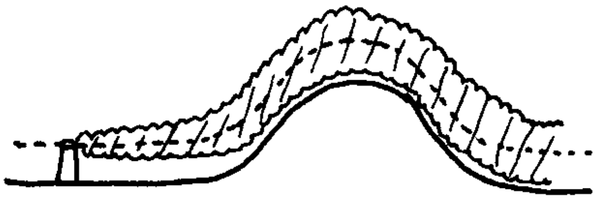
Hydrodynamical models of mountain-valley winds and land-sea breeze effects are available in the literature separate from dispersion models. Again, coupling such models with a dispersion model that can handle complicated wind fields is highly desirable, but the computer times become excessively large.

3.2 The Models

The following paragraphs examine each model individually. Attention has been given to provide an overall picture of the model as well as to focus on some of the unique features, subroutines, parameterizations and limitations. Table 6 is an attempt to summarize in tabular form some of the general characteristics of the models including basic type, geographical



a) a hill in a Gaussian plume-
flow assumed horizontal



b) a hill in a Gaussian plume -
flow assumed parallel to the surface

c) a more realistic possibility
-includes possibility of an eddy in lee of hill
-should include flow around the hill

Figure 8. Effects of Topography on a Plume

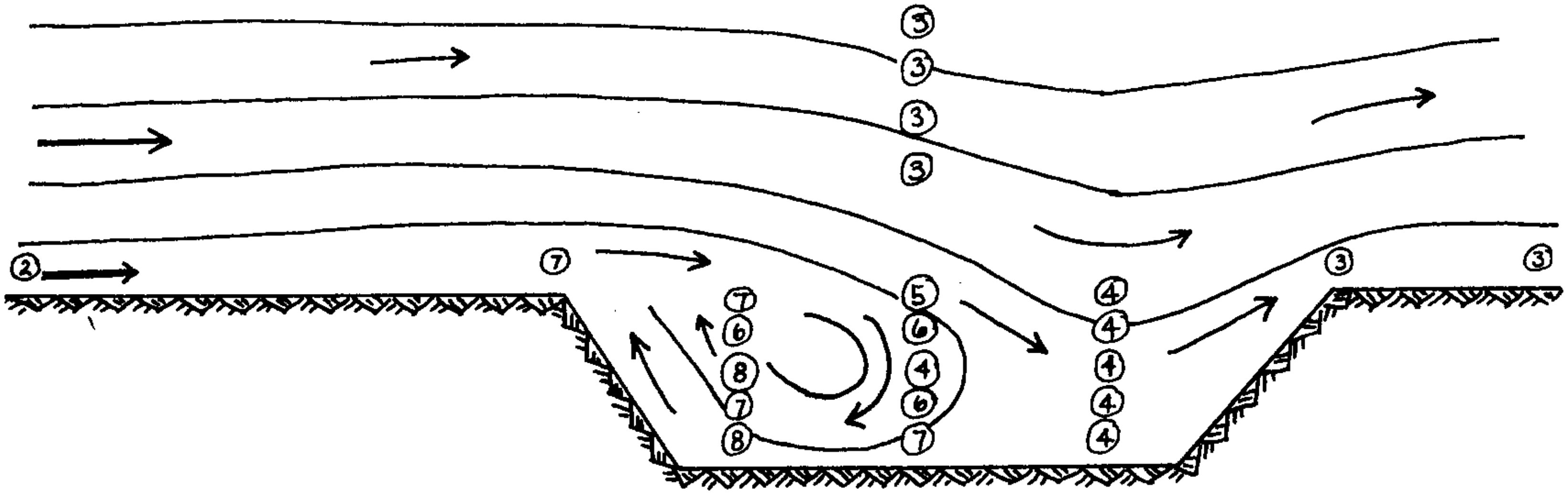


Figure 9. Split flow. The formation of an eddy in a depressed section of highway. Arrows represent winds, numbers represent possible pollution concentrations in arbitrary units.

scope, indication of validation studies that have been carried out, and some estimate of the computer 'costs' (either in dollars per run or in computing time) where this information was available. Table 7 examines the more specific details of each model such as emissions and meteorological parameterizations, and some specific weaknesses and strengths.

The model discussions have been divided into three parts: urban models, highway models, and models available on the Environmental Protection Agency's computer network.

3.21 Urban Models

Although urban models do not pertain directly to highway air quality problems, they may be a better way to go about modeling the effects of a highway in an urban area where there are many other sources and often other roadways. Furthermore, some of these models incorporate features that might be of interest to include in a model of smaller geographical scope.

LAWRENCE LIVERMORE LABORATORY (L.L.L.)

This model is a multi-box air pollution model based on a numerical solution to the conservation of mass equation:

$$\frac{\partial c}{\partial t} = K_h \left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right] + \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) \qquad (17)$$

where the equation has been transformed to a coordinate system following the trajectory of the parcel of emitted gases through a set of fixed boxes. The eddy diffusion coefficients are functions of space and time. Sources and sinks due to deposition are allowed as well as 'leaky' inversions.

The boxes are set up in a way to include topography; that is, the bottom of the box is assigned the height of the average topography of that area. The top of the box is the height of the inversion above the ground

Table 6. General classification of models.

Model Developed by	Name	Basic Type	Applications	Geographical Scope	Cost to Run	Validation
Argonne National Lab.	-	Gaussian puff	highway airport urban	1 km 100 km	-	O'Hare airport Chicago area
Robert G. Lamb & Morris Neiburger	-	Gaussian puff	urban	100 km	-	L. A. Basin
Lawrence Livermore Lab.	-	Multi-box mass conservation	urban region	100 km	-	S. F. Bay area fluorescent particle release
Danard Univ. of Waterloo	-	mass conservation	highways	1 km	10 minutes on ? computer	22 cases at an intersection
INTERCOMP	-	mass conservation	urban, buildings, highways	.5km to 10km variable	1 minute on CDC 6600	Chicago-comparison with data, Argonne 6 highway cases for EPA
AeroVironment	-	Gaussian puff	highways	1 km	minimal	San Jose freeway
Shieh IBM	-	Gaussian plume	urban	50 km	15 sec on an IBM 360/91	2 day's data for New York City
The Research Corporation	-	Gaussian plume	highways	1 km	moderate to little	Hartford, Connecticut freeways
Turner	-	Gaussian plume	general	1-100 km	small	-

Table 6 (continued)

Model Developed by		Basic Type	Applications	Geographical Scope	Cost to Run	Validation
Tio C. Chen & Frederick March	-	Sutton's equation (Gaussian plume in form)	highways	1 km	little	none at time of report (1971)
California Highway Department	-	Gaussian plume	highways	.1-1 km	low tables available	smoke candle studies other validation in progress
Stanford Research Institute	APRAC-1A	Gaussian plume	urban	1-100 km	little	San Jose, St. Louis areas
John R. Zimmerman EPA	HIWAY	Gaussian plume	highways	1 km	little	in progress
General Research Corporation	DIFKIN	mass conservation	urban	100 km	moderate	Los Angeles Basin
	LAPS	mass conservation	highways	10 km	little	Santa Barbara freeway
ESL, Inc.	-	Gaussian plume	highways	1 km	little	in progress
Gifford and Hanna	-	area source (Gaussian plume)	urban	100 km	little	compared with models of Martin & Tikvart, Fortak, Lamb
CEM	-	mass conservation	urban	100 km	large	Los Angeles Basin
System, Science, and Software	PICK	mass conservation	urban	100 km	large	Los Angeles Basin
Hilst	-	Gaussian plume	urban region	100 km	moderate	Connecticut SO_2
Math. Sciences NW	-	Gaussian plume	highway	1 km	little	I-5

Table 7. Specific model characteristics.

Model Developed By	Application	Characteristics	Emissions Model	Meteorological Parameterization	Weaknesses	Strengths
Argonne National Lab.	highway urban	Gaussian puff - line source for skewed winds - point source for parallel	cold start - hot start modes, trucks vs. cars	mean wind $\overline{u}$	-	variable width of highway, inclined highway, varying inversion height
Robert G. Lamb & Morris Neiburger	urban	generalized Lagrangian Gaussian puff, point, area, line sources	source inventory	wind speed & direction as functions of space and time, K's also variable	-	handled background concentrations, some photochem.
Lawrence Livermore Lab.	urban	multi-box mass conservation model with detailed wind field, vertical profiles of velocity and diffusivity	source inventory and assumed daily cycle	mass continuity model - velocity as a function of space and time K's also variable	needs lots of iterations to get wind field	allows 'leaky' inversion, settling velocities, some photochem. topographic effects in wind field
Danard Univ. of Waterloo	highways	mass conservation for a vertical plane perpendicular to highway - an unsteady area source is assumed for highway	emissions same for all cars	K's distributed in log-linear way in vertical, winds vary in time and in vertical	-	variable K's and winds
INTERCOMP	highways urban	mass conservation solved by finite difference scheme steady or unsteady solutions available	-	wind field calculated by potential flow also power law dependence of velocity, K with height	-	K's treated as calibration factors wind field, boundary conditions allow topographic variation
AeroVironment	highways	Lagrangian Gaussian puff model for an unsteady line source, also point sources	based on California Air Quality Manual	roughness reduced wind speed, K's determined from measurements of heat flux, roughness, wind shear	no form for case parallel to highway	wind shifts allowed, inclined highway, applicable for all wind speeds, handles non-uniform spatial dispersion

Table 7 (continued)

Model Developed By	Application	Characteristics	Emissions Model	Meteorological Parameterization	Weaknesses	Strengths
Shieh IBM	urban	Gaussian plume point and area sources handles inversions	source inventory of annual emissions	mean wind, stability classes by Pasquill	annual emissions converted to hourly	requires small amount of computer time
The Research Corporation	at-grade highways	Gaussian finite line source → point source for parallel winds steady state solution	from traffic counts - model to predict traffic flow volumes and speeds, EPA factors	mean wind, stability classes by Pasquill		
Tio C. Chen	highways depressed and elevated	Gaussian point source - series of moving points used to approximate a line	none discussed	generalized eddy diffusion coefficients expressed as functions of wind gustiness	oblique winds not allowed in depressed case	considers depressed highways can handle light wind cases
California Highway Department	highways	Gaussian line source with mechanical mixing cell - point source for parallel winds	based on data for emissions in different modes of travel	mean wind, σ's modified from those of Pasquill to estimate dispersion close to highway	does not handle very light winds	easy to use
Hilst	urban	Gaussian plume point and area sources	source inventory	winds vary in space and time	-	decay factor
Stanford Research Institute	urban	Gaussian plume with extra urban diffusion and building canyon submodels	traffic volume and speed data emissions factor a function of speed	mean wind constant over area σ_y, σ_z from Pasquill-Gifford curves	winds not usually constant over an urban area	building canyon model is unique, gives urban wide patterns
EPA	highways	Gaussian plume - line source as sum over point sources	EPA with Rose correction factors for speed	mean wind, stability class, σ_y, σ_z from Pasquill-Gifford curves	does not treat light wind cases or elevated sections	

Table 7 (continued)

Model Developed By	Application	Characteristics	Emissions Model	Meteorological Parameterization	Weaknesses	Strengths
General Research Corporation	urban highway	semi-Lagrangian moving all mass conservation model	from traffic counts and average speeds	trajectories projected backward in time from receptor	needs high resolution data for validation including NO, NO_2, O_3 measurements	includes photochemistry - no artificial diffusion
ESL, Inc.	highway	Gaussian plume - highway treated as vertical strip source, mixing cell used	-	mean wind speed and direction measured σ_y, σ_z	light wind cases are not handled	includes some photochemistry, % of reflections at ground
Gifford and Hanna	urban	Gaussian plume - modified to give a simple formulation for area sources	source inventory	mean wind and stability	not good for large point sources or detail near a highway	gives reliable estimate to test background effects of general upwind sources
CEM	urban	mass conservation - finite difference solution in Eulerian frame	source inventory and traffic data from Roth, et al.	solves equations of motion, energy and continuity for the atmosphere	requires large amounts of computer time - artificial diffusion was a problem	includes topographic effects
S^3	urban	mass conservation - particle-in-a-cell, semi-Lagrangian approach	traffic data, source inventories	trajectories are used K's are treated as a turbulent flux velocity and are included in trajectory	needs lots of particles to be followed - requires lots of computer storage	gives urban-wide patterns of pollution can be coupled to chem. reaction schemes
Turner	urban or highway	Gaussian plume	none	stability wind rose	-	-
Math. Sciences NW	highway	Gaussian plume - sum over point sources	EPA	stability wind rose	-	-

(this is allowed to change with time). Photochemical reactions where the rate of formation or destruction is proportional to the first power of the concentration are readily handled.

Topography is also included in the wind field calculation. Observations of wind speed, direction and inversion height are obtained from several stations within the region. These values are used to construct a wind system on the grid of the boxes. This wind field is then adjusted so that mass is conserved. If this last step is not done pollution concentrations can build up where the winds tend to converge unnaturally.

A daily averaged source inventory is used for emissions and multiplied by a function approximating the daily cycle.

Tests comparing this model to the analytical solutions show that there is little if any 'artificial diffusion'. Tests in the San Francisco Bay Area with fluorescent tracer releases also show reasonable correlations between measured and observed concentrations.

This model has been especially designed to handle regional scale transport problems. Although it would not be applicable for predicting local effects of a freeway, the impact of a highway network on the entire urban area could be assessed.

SYSTEMS, SCIENCE, AND SOFTWARE (S^3)

The particle-in-cell approach to numerically solving the mass conservation equation was developed primarily by the group at Systems, Science, and Software. In this scheme the terms $\partial/\partial x\ (K_x \partial c_i/\partial x)$, etc. in equation (1) have been transformed by defining a fictitious velocity $u' = \frac{K_x}{c}\partial c_i/\partial x$ to characterize the turbulent flux. When this is done also assuming a non-divergent mean velocity, the basic equation reduces to equation (11). Lagrangian particles are used to represent the pollutant mass. These particles move through a grid of Eulerian cells under the combined influence of the mean wind and the turbulent flux velocity. Boundary conditions determine the losses through the inversions, reflection or adsorption at ground level, and fluxes from (or into) other urban areas. Patterns of pollution concentrations are generated requiring, however, that large numbers of mass particles must be followed. Calculations done for carbon monoxide in the Los Angeles Basin give good agreement with the data.

The dispersion model has been coupled with a photochemical model based on the lumped parameter technique of Eschenroeder and Martinez. Cases were studied again for L.A., where concentrations for NO, NO_2, HC, O_3, and HNO_3 were calculated. More work, especially in specifying the chemical reaction mechanisms was indicated.

THE CENTER FOR THE ENVIRONMENT AND MAN, INC. (CEM)

This extensive three-dimensional model is designed to calculate pollution concentrations in the air and in bodies of water. The main emphasis is on specifying the meteorological conditions in detail. The temperature distribution in the atmosphere is calculated based on the absorption of solar and infrared radiation by water vapor, carbon dioxide, and aerosols. The turbulent equations of motion, the energy equation, the continuity equation, and the humidity equation are used to give the velocity and humidity distributions in the horizontal and vertical. Similar equations are solved in the water (a lake or ocean near the urban area) again to specify flow patterns in the horizontal and vertical. Topographic variations are explicitly included. The eddy diffusion coefficient is a specified function of the Richardson number, Ri (which is an indication of stability and wind shear) and of height. The prediction equation for pollutants:

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial z}\left(K_z\ (Ri,z)\ \frac{\partial c_i}{\partial z}\right) + S_i \qquad (18)$$

is solved by finite difference techniques.

Sensitivity studies were undertaken to examine the effects of the wind calculations, the topographic effects, and land-water effects. The Los Angeles Basin was used for the tests and the model was compared to the models of Roth, et al. (Systems Applications, Inc.) and Sklarew, et al. (Systems, Science, and Software). An emissions inventory was used to prescribe the sources and emissions rates. The best comparisons with the observed CO data occurred where the terrain effects were most important. The wind and humidity calculations looked quite reasonable. The effects of the presence of the ocean were noticeable. The model predicts regional patterns, but so far the computer time requirements are large. It is of interest that this is the only model reviewed here that uses such extensive meteorological calculations and predicts the specific humidity distributions. The humidity distribution, is seen to play an increasingly important role in some of the air chemistry reactions.

LAMB AND NEIBURGER

The model developed at UCLA is generally classed as being of the Gaussian puff type, but actually is quite a bit more general than the commonly used puff models. Equation (1) is set in Lagrangian coordinates, K's are assumed constant in space, but not in time, vertical velocity is zero so there are horizontal motions only, the chemical reaction term is proportional to the concentration and loss is allowed at the ground. The analytical solution obtained is in terms of Green's functions. Area, line, and point sources are modeled. An initial pollutant distribution is specified.

The model has been applied to the Los Angeles Basin. An emissions inventory is used for area and point sources. The freeway network is divided into a series of line source segments. Emissions for freeways are based on traffic count data and average speed for each hour.

The winds are determined from streamline-isotach charts constructed from mean wind observations over the area. Topographic effects are not explicitly included but they influence the two-dimensional flow patterns to some extent. Photochemical reactions of first order are handled in the basic model. Recent work done especially by Lamb has been in improving trajectory analyses and examining how best to include chemical reactions of higher order.

STANFORD RESEARCH INSTITUTE (S.R.I.) - APPRAC-1A

The model developed for the Environmental Protection Agency by the group at Stanford Research Institute is based on the Gaussian plume model. It is an urban model specifically for predicting air quality at specific receptors from highway networks. A system of line sources is set up to match highway networks. The length, end points, peak traffic volumes and type of road (or average vehicle speed) are input to the model. The emissions factor is a function of expected mix of vehicle model years and average speed.

The concentration at a receptor is determined by emissions in an angular segment aligned with the mean wind. Effects of contributions from sources near the receptor are specified in more detail and a submodel includes the effects of vortices set up in building canyons. Contributions from other cities are approximated. Mixing heights are calculated from radiosonde observations. When the plume intersects the mixing height the pollutant is assumed to be distributed uniformly with height. The vertical σ is specified as a function of stability class and downwind distance, similar to Pasquill's formulation.

The building canyon submodel is interesting in that it is an empirical solution to a problem of split-flow. Similar studies in depressed sections of highway with sloping walls might provide the basis for a similar submodel to better predict the air dynamics and hence the pollution concentrations in the immediate vicinity of a roadway.

SHIEH

This urban model predicts SO_2 concentrations using Gaussian plume formulas. Both point sources and area sources (a numerical integration over many point sources) are modeled. Cancawe's plume rise equation is used and the ground is assumed to reflect the pollutant perfectly. The sources and meteorological conditions are allowed to vary in space and time. Two-hour averaged emissions are estimated from annual emissions values using a formulation developed by Shieh. Studies using data from New York City showed qualitative agreement between observed and calculated values.

HILST

The regional air quality model developed by the Travelers Research Center is mainly for SO_2 emissions and so is not directly transportation oriented. It is reviewed here because of the refinements made to the basic Gaussian plume form and because of the sensitivity studies done on the model.

The model calculates ground level concentrations for a 100 kilometer square area at hourly intervals. Gaussian point and area source formulations are used including an exponential decay factor which allows the specification of a half-life or residence time for the pollutant. Meteorological conditions may vary in space but change in time only every other time step (every 2 hours). The wind flow field must maintain mass continuity. To determine the concentration at a receptor a backward trajectory is examined and contributions from sources in this segment are summed.

Sensitivity studies were carried out to determine the effects of errors in source emission rates, decay time, σ_y, σ_z, and wind direction. Comparison of computed and observed values pointed to means of calibrating a model.

GIFFORD-HANNA

The model used by Gifford and Hanna at the Atmospheric Turbulence and Diffusion Laboratory (ATDL) is a simplified formulation to represent area sources. The concentration c is equal to the source strength, Q, divided by the wind speed, u, times a factor M which is a function of stability and can be related to σ_z or K_z.

$$c = M \frac{Q}{u} \tag{19}$$

M ranges from 60 to 600 with an average of 225 corresponding to Pasquill's D stability. This very simple relation allows many possibilities for modification. An early version included in M power law distributions for u and K_z in the vertical. Point sources of the Gaussian plume type are used for large single sources and for sources close to receptors. This model was compared with models of Martin and Tikvart, Fortak for SO_2, and Lamb for CO, all models of greater complexity. The Gifford-Hanna model compared well with the Martin and Tikvart, and Fortak models. The one of Lamb for L.A. included a more careful specification of wind systems which appeared to be important for that case.

The model is simple enough to use for order of magnitude calculations. Formulations are easily derived for dry deposition in terms of a deposition velocity v_a and for precipitation scavenging with an appropriate coefficient Λ. Extensions to handle photochemical reactions of arbitrary order have also been tried with some success.

3.22 Highway Models

The following models have either been developed primarily for use in predicting air quality near a highway or at least have been applied to highway problems in their applications.

INTERCOMP

Another type of mass conservation model is in use at INTERCOMP. The advection-diffusion partial differential equation is solved by finite difference methods. K_x, K_y, K_z are required input to the model and are allowed to vary in space. It is not clear whether the K's are allowed to vary in time in the cases they have considered but the model could handle these cases readily. Time dependent and steady state solutions are available. Only first order chemical reactions have been attempted so far. The only limitations it would seem to the handling of non-linear chemistry terms would be if the finite difference scheme became instable. The computer program is large enough that running solutions for several pollutants to test the effects of chemical reactions would make computer times prohibitively long and expensive. Topographic modeling is present in the wind field calculation and in the K values which can be set to zero at the lower boundaries.

The wind flow pattern is calculated using a modified three-dimensional velocity potential function that allows for flow around and over obstacles like buildings and hills. The modifications are the inclusion of functions which allow $\overline{U}$ to vary with height by a power law or a logarithmic form. The wind speed and eddy diffusivities may vary with height, but the wind direction does not vary (it does in the atmosphere). Eddies in the lee of buildings or in cut sections so far are not predicted but the current work at INTERCOMP is to solve the complete Navier-Stokes equations or at least use them to predict when split flow could occur and how important it may be.

The model has been compared to the Gaussian plume formulation. It was found that the power law variations of K's and $\overline{U}$ with height were necessary to make the predictions compare favorably. Values for the two power law forms have been found that relate the $U(z)$, $K(z)$ to the Pasquill-Gifford stability classes. Thus, this model can accept the simpler input data of Gaussian plume models when more complex meteorological data is not available.

The model has been applied to the Chicago region and compared to the Argonne model with good results. It has also been applied to flow around buildings as seen in wind tunnel studies and was tested by EPA to predict concentrations downwind of at-grade highways and cut sections.

DANARD, ET AL.

Another mass conservation model for highway air quality prediction was developed at the University of Waterloo, Ontario, Canada. A two-dimensional, time-dependent diffusion equation is integrated by finite difference techniques:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} (K_x \frac{\partial c}{\partial x} - cu) + \frac{\partial}{\partial z} (K_z \frac{\partial c}{\partial z}) \qquad (20)$$

A vertical plane perpendicular to the highway is considered. K_x and K_z are assumed to be functions of height, wind speed measured at 10 meters height, roughness length, and distance from the highway. Upper boundary conditions for K_z and K_x are determined from the sign of the temperature advection aloft. The wind speed varies logarithmically with height up to 10 meters and linearly with height up to the measured mixing height. The equation is integrated until the flux through the downwind boundary equals the input from the vehicle emissions. Emissions are specified as mass per car. No speed or model year factor is included.

Comparison of predicted results with observations taken at a fixed site showed an underestimate of the CO concentrations. Specification of background contributions would have increased the accuracy of the predictions.

GENERAL RESEARCH CORPORATION (GRC)

Eschenroeder and Martinez working at General Research Corporation have developed two models of interest. The first model applies to an urban area. Equation (12) is solved in the Lagrangian frame of reference by finite difference techniques for the Los Angeles Basin. The source terms are the chemical rate equations solved simultaneously with the diffusion equations for the reactive species. The set of reactions modeled is presented in Table 4. Source inventories by the Los Angeles Air Pollution Control District and one developed by Systems Applications, Inc. have been used to estimate emissions in the Eulerian grid by automotive and non-automotive sources. Meteorological conditions are specified by inversion heights and trajectories. The trajectories are traced backwards in time from the receptor using nearby observations compiled by the Scott Research Laboratory.

The model developed for roadways is of particular interest. Equation (13) is used, where dispersion in the y direction may be handled analytically giving a Gaussian distribution. The rest of the equation is solved by numerical techniques. High space and time resolution are possible for winds at all angles to the road. Emissions are given in terms of vehicle speed and volume and must be specified for each pollutant. A simplified chemical reaction set is used assuming that O_3, NO, and NO_2 come quickly into equilibrium with the amount of sunlight (first three reactions of Table 4). Adsorption is allowed at the ground. Several kinds of highway configurations are allowed (depressed, at-grade, elevated on landscaped fill, and elevated structures). The diffusion coefficients are varied to account for the locally enhanced eddy diffusivity because of turbulent mixing in the wakes of vehicles. Computer time is quite reasonable for this simple formulation. The more detailed chemical kinetics may be necessary where the polluted air remains over the highway for some time as in the parallel wind condition.

ARGONNE NATIONAL LABORATORY

This group has developed essentially two models. The urban model has been applied to SO_2 and CO. Area sources and point sources are considered in the context of a time dependent Gaussian puff model. Reflection at the gound and from inversions aloft is included. Virtual sources are used to model the dispersion. Trajectories of air parcels passing over a receptor are determined from wind speed and direction measurements from the nearest observing station. For the CO study of the Chicago area detailed traffic information was obtained and an emissions model including the additional effects of cold start emissions was developed. Emissions were then specified for each grid square.

The highway/airport model developed more recently again adopts the Gaussian puff model concepts, but the puff is extended to model a finite length line. No ground reflection was assumed for the testing of the model. The angle between the wind vector and the highway is used to set up three regimes of the model. For nearly perpendicular winds the crosswind formulation (which has angular dependence included) is used. For intermediate winds, θ between 30° and 10°, the line source is broken into smaller segments and the crosswind formulation is applied to each. For θ less than 10° the parallel wind solution (the limiting value of the crosswind as $\theta \to 0$) is used. The effects of an inclined line has also been modeled. Mean wind speeds and directions were used and σ_y and σ_z were calculated as functions of downwind distance, presumably from Pasquill-Gifford curves. Validation studies were conducted at O'Hare airport for NO_x.

AEROVIRONMENT, INC.

This model is of the Gaussian puff type. The basic equation is transformed to the Lagrangian frame of reference. Eddy diffusion coefficients are expressed as functions of time. The unsteady solutions obtained are for point or line sources and are valid for light winds and calm conditions. Steady-state solutions may also be derived. The case of a skewed line of finite width requires a numerical solution.

The eddy diffusion coefficients are estimated using on-site measurements of temperature, verification of roughness length, and heat flux determined from measured values of solar insulation. Inclusion of the roughness parameter Z_0 allows some distinction between flat terrain and buildings close to the highway. Variable winds are handled by changing them at each time step but assuming constant winds between steps.

This model requires very little computer storage or time. Emissions are input; California factors have in general been used. Background emissions from stationary sources are also included. The model has been validated at two sites along Route 101 in the San Jose area and has been used to predict air quality for Routes 85 and 87 in San Jose.

CHEN AND MARCH

A different approach to modeling the effects of particular highway designs is seen in the equations developed by Chen and March. The basic analytical solution is Gaussian plume in form but was developed by Sutton and the σ's replaced by generalized eddy diffusion coefficients which are functions of downwind distance, kinematic viscosity, gustiness of the wind, and a turbulence coefficient which determines the power law form for the variation of wind speed with height. The moving point source formula is used and summed over each point (or vehicle). Reflection at ground level of a plume emitted from a lane at height h above the ground is used to model elevated sections. Reflection at the ground and at the side walls is used to model depressed highways. Oblique winds for elevated and at-grade highways are divided into the two components parallel and perpendicular to the roadway. Concentrations are calculated for each component and summed. Winds can only be parallel to the depressed highway.

Sensitivity studies were conducted to determine the effects of gustiness, turbulence coefficient, position of the traffic lane in the cut section, and the effects of the side walls. No validation cases had been calculated at the time of the report (1971).

D. B. TURNER

The Workbook of Atmospheric Dispersion Estimates is really a system of models used by many groups to obtain air quality predictions. It's primary use is in considerations of emissions from point sources, but area and line sources are discussed. The basic model is the Gaussian plume. Extensions to area sources, infinite and finite line sources are discussed. Discussions of appropriate σ_y, σ_z values, determination of stability class, and calculation of effective stack height make this workbook a helpful tool. Approximations to handle fumigation and topographic problems are suggested. The limitations of the Gaussian plume model are discussed and example problems are worked.

MATHEMATICAL SCIENCES NORTHWEST

This Gaussian plume model is based on information provided in D. B. Turner's Workbook. A line source is approximated by a series of point sources. Highway networks are mapped by such points so that even curved highways are easily handled. The calculations are subject to a correction factor near the road to compensate for the effect of a series of point sources. Any wind direction can be handled. The meteorological input is wind speed, direction, and Pasquill Stability Class. EPA emissions factors are used. Flat terrain, at-grade highways, and constant wind speed and direction are assumed.*

---

*This model was used by the authors of this review in studies for Mathematical Sciences Northwest, Seattle, Washington, and Environment Resources Associates, Redmond, Washington, on studies of I-90 and I-5 (1972, 1973).

THE RESEARCH CORPORATION OF NEW ENGLAND (TRC)

The Research Corporation (TRC) has developed an air quality model for highways based on the Gaussian finite line source formulation presented in Turner's Workbook. Modifications to the basic formulation include use of a point source for modeling the highway when the winds are parallel, and approximations for other angles. Stability wind roses are used as the meteorological input.

Of special note is the emissions calculation. EPA emissions factors are used. The method of arriving at the traffic volume and speed is of interest. The model varies travel speed and traffic volume based on traffic counts at on and off ramps and a theoretical lane capacity curve. The vehicle speed decreases as traffic volume increases until the speed is about 35 mph. Below this point the speed decreases much more rapidly as the volume continues to increase. At 10 mph traffic jam conditions are assumed and more vehicles enter only when space becomes available. The output of this submodel is traffic volume and vehicle speed for each time segment. Emissions can be specified as a function of time much more carefully using this sort of approach.

CALIFORNIA STATE HIGHWAY DEPARTMENT

The State of California Highway Department has developed their own in-house capability for preparing environmental impact statements with the help of a Gaussian line source model for predicting air quality. The model employs a mixing cell approximation directly over the highway, from shoulder to shoulder and twelve feet in the vertical, to account for the mechanical mixing by the traffic. In this cell the concentration is constant. Smoke candle studies (smoke candles mounted on exhaust pipes) have verified the dimensions of the cell. Beyond this region a Gaussian line source model is used with several different forms depending on highway design, heights of sources and receptors, and parallel or skewed winds.

Stability wind roses are determined from on-site measurements and typical and worst cases are defined. The σ_y and σ_z's used are those of Pasquill-Gifford, but they have been empirically extended to small downwind distances (less than .1 kilometers) to account for dispersion near the source. The emissions factors used are based on measurements of emissions for a test cycle specified by the California Air Resources Board and on the Federal test cycle for city streets. Graphical solutions are available for a specified average speed and vehicle mix.

Effects of topography have not been considered in the basic model nor pursued in field work. Data is available for some highway sections in deep valleys and a mountain pass, but it has not been analyzed.

Solutions to the Gaussian line source model are presented in graphical form so no calculations other than linear interpolations are necessary. The clear presentation of the model discussion of its limitations, and examples make this model readily usable.*

ESL, INC.

The model developed by ESL, Inc. is a refinement of the Gaussian plume model. Equations are developed to treat the case of a roadway as a vertical strip source, where the pollutants are assumed to cross the vertical plane on the lee side of the highway in a strip of height h and width Δh. The values for h and Δh depend on traffic speed, volume, the

---

*Several of the authors of this review have used the California Highway Department's model for calculating pollution concentrations near a highway. The study was done for Richard Carothers Associates, Seattle, Washington, on Highway I-15 in southern Idaho (1973, to be published).

number of lanes, and the atmospheric turbulence. All wind directions are approximated and a variable R is included to allow for varying percentages of reflection of the plume at the ground. The downwind dependence of σ_y and σ_z are based on experimental data and are related to the standard deviations in the lateral and vertical wind directions which are measurable For heavier pollutant particles like lead a term is included to allow for gravitational fall-out.

Chemical reactions are handled by applying the diffusion equations and the finite differenced chemical rate equations alternately using small time steps. This approach assumes that for a short enough time interval the simultaneous processes of diffusion and chemical reaction may be treated as an alternating sequence of pure diffusion and pure chemical transformation. No limit on the order of the reactions is necessary. When the reactions are first order the model reverts to the use of a simple depletion factor.

The dispersion involving chemical reactions is divided into two regimes: one over the roadway where an approximation is used to model the mechanical mixing by the cars, and the second some distance downwind where the plume is again Gaussian.

3.23 EPA Models

The Environmental Protection Agency has established a computer network UNAMAP through which programs are made available to regional offices for the assessment of air quality. The Computer Sciences Corporation has been selected as the commercial outlet where non-EPA users may contract to use EPA models. This network, INFONET, will contain the EPA programs and EPA will assume the responsibility for storing the models, updating the models and model inventory and providing messages to users of changes. Peter Loux of Computer Sciences Corporation is the person to contact (703-527-6080).

As of June 1973, six models are available on UNAMAP: APRAC-1A, HIWAY, CDM, PTMAX, PTDIS, PTMTP.

APRAC-1A

This model, already described above, was developed for EPA by Stanford Research Institute. This model estimates the effects of highways and streets on the urban environment, allowing for diffusion into the area from other cities and taking into account other area source emissions and building canyon effects. This model is recommended for use by the EPA when a highway is to be built or modified in an urban area. Background emissions are handled better in this model than in HIWAY.

HIWAY

HIWAY is the EPA line source model for calculating short term (hourly) concentrations downwind of roadway sources. It is most applicable near the highway; that is, tens to hundreds of meters downwind. The model for at-grade sections considers each lane of traffic as a line source; the cut section is modeled as an area source which is composed of ten line sources positioned at the top of the cut and each given an equal weighting of the emissions from the lanes below. The line sources in both cases are approximated by a numerical integration over a series of Gaussian (plume) point sources. The spacing of these point sources is halved again and again until the integration converges. The line source approximation is valid for winds greater than 10° off of parallel; winds nearly parallel to the highway are handled separately. Mechanical mixing due to the movement of the vehicles is included as an initial vertical and horizontal spreading of the plume (σ_{zo}, σ_{yo}) which can be envisioned as a 'virtual' point source upwind which will give such a spread over the lane being modeled.

The interactive program included in UNAMAP allows the specification of up to twenty-five receptors. The emissions may be specified by the user or those of EPA including correction factors for average speed may be calculated in the program. Zero and light wind categories cannot be handled. The formulation is not recommended for use with elevated sections of highway. This model is being tested this summer (1973) using tracer gases and measured CO data.

CDM

The Climatological Dispersion Model determines long-term (monthly, seasonal, annual) concentration patterns from point and area sources using a comprehensive emissions inventory and stability wind rose data (stability wind rose is a joint frequency distribution of stability, wind speed, and wind direction). This model is primarily applicable to SO_2 and particulate emissions. It is a modified version of the Air Quality Display Model (AQDM) developed by Martin and Tickvart at TRW. The Gaussian plume model was used for point and areas sources with an effective stack height determined from a plume rise equation. The improvements made in the basic model include use of the Briggs' plume rise equation, a different specification of area sources (as an upwind line source), an exponential decay factor (lifetime) is included, and the wind speed is a power law function of height where the exponent is a function of stability.

PTMAX

PTMAX calculates the maximum, 10 minute, ground level concentrations downwind from a single point source as a function of stability and wind speed. The model is based on the Gaussian point source formulas in D. B. Turner's Workbook. Briggs' plume rise equations are used and Pasquill's stability classes and σ_y, σ_z's.

PTDIS

Again based on Turner's Workbook, this model calculates downwind ground level concentrations for various downwind distances for a single point source. Stability, wind speed, and mixing height are the necessary meteorological input. Briggs' plume rise and σ_y, σ_z are used.

PTMTP

This model produces hourly concentrations at up to 30 receptors from multiple point sources (up to 25). The Gaussian plume model again is used following formulas in Turner's Workbook. Three hour to twenty-four hour averages are calculated both as total concentration at each receptor and individual contributions from each source. Stack parameters and meteorological input (stability, wind speed, wind direction, mixing height) are necessary for each hour.

None of these models are applicable to reactive pollutants, situations involving complex terrain, or zero wind cases. Models to handle some of these cases are being developed. A model calculating a worst day case (a 24 hour maximum) in a year based on hourly meteorological data and a real time air quality simulation model for use during stagnation and episode conditions are being developed. Three contracts have been signed for the development of photochemical models for Los Angeles. Other things like cost of control strategy models and rollback models are being discussed.

3.3 Further Models that need to be Reviewed

Response to the request for information has been incomplete as evidenced by Table 1. There are some specific models with unique refinements that should be reviewed before any final decision is made as to which models to use for air quality impact analysis.

In most cases there was a specific reason for contacting particular individuals or organizations. The last column in Table 1 gives some idea of this reason for persons who have not responded.

The dispersion model of North American Weather Consultants which attempts to predict concentration values on the basis of statistical studies should be examined. The meteorological parameterization of the Environmental Research on Technology group which uses Blackadar's wind profiles is of interest. The models developed by Tio Chen including dynamic effects of highways need to be considered. The studies conducted by Systems Applications, Inc. in the Los Angeles Basin look quite interesting. They also have a model for highways which includes photochemistry. The area of air chemistry and topographic effects are really just beginning to be tackled and should be watched closely in the next few years.

It should be noted that there are many places where plume models based on Turner's Workbook are available, certainly more than a dozen places in Washington alone. This study has concentrated on examining model refinements and the diverse types of models not on cataloguing who has what. One of the beauties of the Gaussian plume model is that it is so readily usable.

4.0 GENERAL DISCUSSION

The study reported here and the DOT study clearly indicate that there are a large number of models available for the prediction of the air quality impact of a highway on its environment. The diversity exhibited by these models lies not only in the basic dispersion assumptions used, but in the refinements, the expense to run, the geographical scale each is applicable to, and in the work done to calibrate the models. In some cases it is obvious that one model is better suited to handle a particular situation than another. For example, in a relatively flat area or for short distances and times the Gaussian line source formulation would be quite adequate. On the other hand, in a region of extreme topographic variation, where calm conditions are common, or where split flow may be a significant problem special subroutines may be needed or one of the more complicated models might be necessary.

In light of the above, there are various factors which should be considered when identifying a model (or set of models) for use in air quality prediction. Several of these quantities; emission estimate, traffic flow, meteorological input, photochemistry, and model sensitivity, are discussed briefly below.

The estimation of the emissions is important in that errors included here are reflected in the values obtained for the concentrations downwind. These estimates should be made using the best available models (the Argonne, EPA, or California models appear to be good from this standpoint). Subroutines for predicting traffic flow and for use in particular wind-field - topographic interaction patterns may be required in certain situations which will depend on roadway configuration and the surrounding environment.

The meteorological input is also crucial. Values for wind speeds should be taken on site for best results. Sites where the winds vary little in the horizontal might be a good place for the use of a more simple model such as a Gaussian line source model. In a case where winds at a site are complicated, a mass conservation approach may be necessary. Regions of split flow where eddies may be a problem have been handled in one of three ways, with a complicated model (such as the Intercomp approach), a submodel like the SRI building canyon model, or an empirical model developed with careful studies of actual data.

The need for photochemical models should be assessed in the State of Washington to determine how detailed a model is necessary under "typical" and "worst case" conditions. A model which can incorporate photochemistry may or may not be necessary. Similarly, the need for specifying background concentrations should be assessed as they may contribute significantly to pollution problems for a highway. A model that can accurately incorporate these additional contributions may be necessary especially in urban areas.

The sensitivities of models to different input conditions should be assessed. For example, if a model is not sensitive to the emissions factor a simpler factor may be used without loss of much accuracy. The combination of sensitivity studies, cost-benefit analysis, and on site calibrations should lead to a reliable model or set of models to be used for environmental impact analysis.

An attempt was made to subjectively compare the models analyzed with respect to some of the characteristics mentioned above. The matrix presented in Table 8 assigns a number to each characteristic on a scale from one to three, where one indicates the most desirable, three the least desirable. Where both urban and highway models were developed by one group the highway model was examined. It can be seen that those models which are most flexible and complex tend to be more difficult to use, requiring a larger cost and/or computer capability.

General limits to the applicability of models may be specified, but some limitations can only be seen through use and detailed validation procedures. Studies comparing specific models to air quality data should attempt to clarify these limits to aid highway personnel in assuring correct use of the models.

Table 8. Matrix presentation of the models and various characteristics.

model	allows for variations with time	allows for variations in space	can include background conc.	can include complex sources	can include different highway designs	can include topographic effects	valid in calm or light winds	can include chemical reactions	can include depletion	needs only simple meteorological input	well calibrated	easy to use	small computer sufficient	cost reasonable	especially adapted for highway sources
AeroVironment	1	2	2	2	2	2	1	3	3	1	2	2	2	1	1
Argonne	2	2	2	1	3	3	2	3	3	1	2	1	2	2	2
California H.D.	3	3	3	3	1	3	3	3	3	1	2	1	1	1	1
C.E.M.	1	1	1	1	3	1	1	2	2	3	3	3	3	3	3
Chen	3	3	3	3	1	3	3	3	3	2	3	1	1	1	1
Danard	2	2	3	3	3	3	1	3	3	1	3	2	2	2	1
E.P.A. (HIWAY)	3	3	3	3	1	3	3	3	3	1	2	1	1	1	1
ESL, Inc.	2	3	3	3	3	3	3	1	1	1	2	1	2	1	1
G.R.C.	1	1	1	2	1	2	1	1	1	2	3	3	3	3	1
Gifford/Hanna	3	3	2	3	3	3	3	3	3	1	3	1	1	1	3
Hilst	2	1	1	1	3	2	2	3	2	2	2	3	3	3	2
INTERCOMP	2	1	1	2	1	1	1	2	1	2	3	3	3	2	2
Lamb/Neiburger	1	1	1	1	3	2	1	2	1	3	2	3	3	3	2
L.L.L.	1	1	1	1	3	1	1	2	1	3	3	3	2	2	2
Math. Sciences	3	3	2	1	3	3	3	3	3	1	3	1	1	1	1
Shieh	2	1	2	1	3	3	3	3	3	1	3	2	3	2	3
S^3	1	1	1	1	3	2	1	1	1	3	3	3	2	2	2
S.R.I.	3	3	1	1	3	3	3	3	3	1	2	1	2	1	1
TRC	3	3	3	2	3	3	3	3	3	1	1	1	1	1	3
Turner	3	3	3	2	3	3	3	3	3	1	1	1	1	1	3

5.0 SUMMARY AND RECOMMENDATIONS

The objective of this study has been to conduct a search of the literature to identify state-of-the-art air quality predictive schemes applicable to motor vehicle transportation. These models are necessary for environmental impact statement preparation with regard to highway design and location. The available models were analyzed in detail and evaluated in terms of the selected characteristics that serve to describe the predictive capabilities and limitations of each.

The assessment provided by this report indicates considerable activity is currently underway in the area of highway transportation oriented air quality dispersion models. This activity is characterized by some diversity in approach, scope and scale of work, and model complexity. However, it appears that all models that have been developed have not undergone adequate calibration and verification. Current efforts to test selected models appear promising but it is too early to determine the results of these studies.

Based on the models analyzed, it appears that in most circumstances, on-site parameterization of meteorological, topographical, climatological, and other features is required prior to model application. As a general rule, the more complex the model formulation, the more complex the data and parameterization requirements.

It is recommended that the simplest model that is applicable be used to do the job. A Gaussian plume model in most cases should be quite adequate. In general, these models are valid for short times and short downwind distances and thus are well suited for most highway problems. These models require a minimum of input data and are readily developed for in-house use either in computer form or with generalized results presented in graphical form. Furthermore, the more complex models generally use the Gaussian plume models as a standard with which to compare their results.

The California Highway Department model and EPA's HIWAY, and the Mathematical Sciences Northwest model are the simplest models and are readily available. Since they can handle several highway designs and require only simple meteorological input they are recommended for use. For more complex situations where time and spatial variability of winds and stabilities are a problem or where some topographic variations may influence the wind flow or where calm conditions are prevalent a model such as that of AeroVironment should be considered. This model is simple enough not to require a large computer, yet it can handle some of these more complex problems.

It is further recommended that more complicated models be considered not for immediate use but for future applications if the need for more complex models is shown and provided more complete meteorological and air quality measurements are available for input and verification. Models such as the Lamb and Neiburger model and the General Research Corporation highway model allow for better handling of topographic effects and chemical reactions. (Before a final choice is made some of the models mentioned in section 3.3 should be reviewed.)

It should be kept in mind that with qualified consulting assistance refinements to some of the above models may be possible based on empirical results (like the building canyon model).

Local highway department personnel can be trained to use the simple models. Short training seminars should be arranged for the purpose of discussing the proper methods of collecting data to calibrate the models as well as instruction into some of the physical bases for the models.

Highway personnel should then be able to assess for what situations the simple models are applicable and under what circumstances a more complicated model or special guidance would be necessary.

Serious consideration should be given to selecting or obtaining a staff person or outside consulting assistance to be able to handle cases where the applicability of a simple model might be in question. Such a person or persons should be well-trained in meteorology and be familiar with the various computer models to use as alternatives.

Any model selected for general use and models to be available to handle more difficult situations must be carefully validated by collecting and analyzing applicable air quality and meteorological data. Thus it is recommended that the Washington State Department of Highways undertake a field-oriented research project designed to evaluate the performance of selected atmospheric diffusion models, to determine their applicability to the field of motor vehicle transportation. Such a study would constitute the initial calibration of the models to Washington state conditions. At the same time the models' sensitivity to the input parameters should also be examined.

Cooperation with the EPA research groups and the California highway department research group with respect to data collection and standardization is essential. Such cooperation could speed the model validation and increase the confidence in the use of the validated models.

Implementation of the above recommendations would provide the tools and resources for assessing the potential impact on air quality from proposed highway developments, and thus provide opportunities for minimization of undesirable environmental effects through better location and design.

6.0 REFERENCES

Anon. 1972: Air Quality Analysis and Impact Study of Routes 85 and 87 in the San Jose Area, AerVironment, Inc., Pasadena, California Report AV FR 232, November, 1972.

Anon. 1972: Air Quality Model for Roadways, General Research Corporation Report, December, 1972.

Anon. 1973: Air Quality Studies at General Research Corporation, General Research Corporation Report, June, 1973.

Anon. 1972: Description of Computer Codes for Air Pollution Modeling, General Research Corporation Report, February, 1972.

Anon. 1972: ESL, Inc. Report ESL-Q870, Exhibit A.

Beaton, J. L., A. J. Ranzieri, J. B. Skog, 1972: Air Quality Manual: Vol. I: Meteorology and Its Influence on the Dispersion of Pollutants from Highway Line Sources. Department of Transportation Report FHWA-RD-72-33.

Beaton, J. L., A. J. Ranzieri, J. B. Skog, 1972: Air Quality Manual: Vol. II: Motor Vehicle Emission Factors for Estimates of Highway Impact on Air Quality. Department of Transportation Report FHWA-RD-72-34.

Beaton, J. L., E. C. Shirley, J. B. Skog, 1972: Air Quality Manual: Vol. III: Traffic Information Requirements for Estimates of Highway Impact on Air Quality. Department of Transportation Report FHWA-RD-72-35.

Beaton, J. L., A. J. Ranzieri, E. C. Shirley, J. B. Skog, 1972: Air Quality Manual: Vol. IV: Mathematical Approach to Estimating Highway Impact on Air Quality. Department of Transportation Report FHWA-RD-72-36.

Beaton, J. L., A. J. Ranzieri, E. C. Shirley, J. B. Skog, 1972: Air Quality Manual: Vol. V: Appendix to Vol. IV. Department of Transportation Report FHWA-RD-72-37.

Beaton, J. L., A. J. Ranzieri, E. C. Shirley, J. B. Skog, 1972: Air Quality Manual: Vol. VI: Analysis of Ambient Air Quality for Highway Projects. Department of Transportation Report FHWA-RD-72-38.

Beaton, J. L., E. C. Shirley, J. B. Skog, 1972: Air Quality Manual: Vol. VII: A Method of Analyzing and Reporting Highway Impact on Air Quality. Department of Transportation Report FHWA-RD-72-39.

Beaton, J. L., J. B. Skog, 1972: Air Quality Manual: Vol. VIII: Synthesis of Information on Highway Transportation and Air Quality. Department of Transportation Report FHWA-RD-72-40.

Black, J. F., 1972: You Can Forecast CO Concentrations. The American City, June, 1972, pp. 71-75.

Calder, K. L., 1972: Air Pollution Concentrations from A Highway in an Oblique Wind, EPA, Division of Meteorology, Research Triangle Park, N. C., August, 1972.

Chen, T. C., F. March, 1971: Effect of Highway Configurations on Environmental Problems--Dynamics of Highway Associated Air Pollution, in Proceedings of the Second International Clean Air Congress, Academic Press, 1971, pp. 35-40.

Croke, E. J., K. G. Croke, J. E. Norco, 1972: The Role of Transportation Demand Models in the Projection of Fugure Urban and Regional Air Quality, Argonne National Laboratory, Center for Environmental Studies, June, 1972.

Dabberdt, W. F., F. L. Ludwig, W. B. Johnson, 1971: Urban Diffusion of Carbon Monoxide in Proceedings of the Symposium on Air Pollution, Turbulence and Diffusion, December 7-11, 1971, pp. 145-151.

Dabberdt, W. F., F. L. Ludwig, W. B. Johnson, Jr., 1972: Validation and Applications of an Urban Diffusion Model for Vehicular Pollutants, Stanford Research Institute, Menlo Park, California, December, 1972.

Danard, M. B., R. S. Koneru, P. R. Slawson, 1971: A Numerical Model for Carbon Monoxide Concentrations Near a Highway, in Proceedings of the Symposium on Air Pollution, Turbulence and Diffusion, December 7-10, 1971, pp. 152-157.

Darling, E. M., Jr., 1972: Computer Modeling of Transportation--Generated Air Pollution: A State-of-the-Art Survey, Department of Transportation Report DOT-TSC-OST-72-20.

Dickerson, M. H., 1973: A Mass-Consistent Wind Field Model for the San Francisco Bay Area, Lawrence Livermore Laboratory Report UCRL-74265.

Eschenroeder, A. Q., J. P. Martinez, 1972: Concepts and Applications of Photochemical Smog Models. Advances in Chemistry, vol. 113, pp. 101-168.

Eschenroeder, A. Q., J. R. Martinez, R. A. Nordsieck, 1972: Evaluation of a Diffusion Model for Photochemical Smog Simulation, General Research Corporation Report CR-1-273, October, 1972.

Gifford, F. A., Jr., S. R. Hanna, 1970: Urban Air Pollution Modelling, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 37, December, 1970.

Gifford, F. A., Jr., 1972: Atmospheric Transport and Dispersion over Cities, Nuclear Safety 13 (5), 591-402.

Gifford, F. A., 1972: Applications of a Simple Urban Pollution Model, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 68, October, 1972.

Gifford, F. A., S. R. Hanna, 1973: Modelling Urban Air Pollution, Atmospheric Environment 7, 131-136.

Hanna, S. R., 1971: A Simple Method of Calculating Dispersion from Urban Area Sources, Journal of the Air Pollution Control Association 21 (12), 774-777.

Hanna, S. R., 1972: Description of ATDL Computer Model for Dispersion from Multiple Sources, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 56, April, 1972.

Hanna, S. R., 1972: A Simple Model for the Analysis of Photochemical Smog, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 69, October, 1972.

Hanna, S. R., 1972: Dry Deposition and Precipitation Scavenging in the ATDL Computer Model for Dispersion from Multiple Point and Area Sources, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 71, October, 1972.

Hanna, S. R., 1973: Application of a Simple Dispersion Model to a Rural Industrial Region, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 77, March, 1973.

Hecht, T. A., J. H. Seinfield, 1972: Development and Validation of a Generalized Mechanism for Photochemical Smog, Environmental Science and Technology 6, p. 47.

Hilst, G. R., 1970: Sensitivities of Air Quality Prediction to Input Errors and Uncertainties, in Proceedings of Symposium on Multiple-Source Urban Diffusion Models, Air Pollution Control Office Pub. No. AP-86, pp. 8-11.

Johnson, W. B., 1972: The Status of Air Quality Simulation Modeling, Proceedings, Interagency Conference on the Environment, Lawrence Livermore Laboratory, Livermore, California, October, 1972, 17-19.

Knox, J. B., R. Lange, 1972: Surface Air-Pollutant Concentration Frequency Distributions: Implications for Urban Air Pollution Modelling, Lawrence Livermore Laboratory Report UCRL-73887.

Knox, J. B., R. I. Pollack, 1972: An Investigation of the Frequency Distributions of Surface Air-Pollutant Concentrations, Lawrence Livermore Laboratory Report UCRL-74063.

Knox, J. B., 1973: Numerical Modelling of the Transport, Diffusion and Deposition of Pollutants for Regions and Extended Scales, Lawrence Livermore Laboratory Report UCRL-74666.

Lamb, R. G., M. Neiburger, 1971: An Interim Version of a Generalized Urban Air Pollution Model, Atmospheric Environment, 5, 239.

Lamb, R. G., 1971: The Application of a Generalized Lagrangian Diffusion Model to Air Pollution Simulation Studies, in Proceedings of the Symposium on Air Pollution, Turbulence and Diffusion, December 7-10, 1971, pp. 352-359.

Lamb, R. G., J. H. Seinfeld, 1973: Mathematical Modelling of Urban Air Pollution: General Theory, Environmental Science and Technology 7 (3), 253-261.

Lamb, R. G., 1973: Note on the Application of K-theory to Diffusion Problems Involving Nonlinear Chemical Reactions, Atmospheric Environment 1, 257-263.

Lantz, R. B., K. H. Coats, C. V. Kloepfer, 1971: A Three-Dimensional Numerical Model for Calculating the Spread and Dilution of Air Pollutants, in Proceedings of the Symposium on Air Pollution, Turbulence and Diffusion, December 7-10, 1971, pp. 43-49.

Lantz, R. B., R. C. McCulloch, R. K. Agrawal, 1972: The Use of Three-Dimensional Numerical Air Pollution Models in Planning Plant Location. Design and Operation. The Journal of Canadian Petroleum Technology, July-September, 1972, Montreal, pp. 1-8.

Lissaman, P. B. S., 1973: A Simple Unsteady Concentration Model Explicitly Incorporating Ground Roughness and Heat Flux, Aerovironment Report #73-129, 1973.

Ludwig, F. L., W. F. Dabberdt, 1972: Evaluation of the APRAC-1A Urban Diffusion Model for Carbon Monoxide. Final Report, Coordinating Research Council Contract CAPA-3-68 (1-69), Stanford Research Institute, Menlo Park, California, 115 pp.

Ludwig, F. L., R. C. Sandys, A. E. Moon, 1972: Preliminary Studies of the Modelling of Air Pollution Effects from Traffic-Engineering Alternatives. Stanford Research Institute, Menlo Park, California, August, 1972.

Ludwig, F. L., W. F. Dabberdt, 1973: Effects of Urbanization on Turbulent Diffusion and Mixing Depth. Stanford Research Institute, Menlo Park, California.

MacCracken, M. C., T. V. Crawford, K. R. Peterson, J. B. Knox, 1971: Development of a Multi-Box Air Pollution Model and Initial Verification for the San Francisco Bay Area, Lawrence Livermore Laboratory report UCRL-73348.

MacCracken, M. C., T. V. Crawford, K. R. Peterson, J. B. Knox, 1972: Initial Application of a Multi-Box Air Pollution Model to the San Francisco Bay Area, Lawrence Livermore Laboratory report UCRL-73944.

MacCready, P. B., Jr., Use of Monostatic Acoustic Radar for Low Level Diffusion Studies, AeroVironment Memorandum #AV-M-312, 1973.

Mahoney, J. R., B. A. Egan, 1971: A Mesoscale Numerical Model of Atmospheric Transport Phenomena in Urban Areas in Proceedings of the Second International Clean Air Congress, Academic Press, 1971, pp. 1152-1157.

Mancuso, R. L., F. L. Ludwig, 1972: User's Manual for the APRAC-1A Urban Diffusion Model Computer Program. Report, Contract CAPA-3-68 (1-69), Stanford Research Institute, Menlo Park, California, 119 pp.

Martinez, J. R., R. A. Nordsieck, A. Q. Eschenroeder, 1973: Impacts of Transportation Control Strategies on Los Angeles Air Quality. General Research Corporation Report CR-4-273, May, 1973.

Moon, A. E., F. L. Ludwig, 1973: Predicting Motor Vehicle Air Pollution Concentrations from Highway Network Analysis. Stanford Research Institute, Menlo Park, California, January, 1973.

Pandolfo, J. P., C. A. Jacobs, 1973: Tests of an Urban Meteorological-Pollutant Model Using CO Validation Data in the Los Angeles Metropolitan Area, Volume I, The Center for the Environment and Man Report 490a.

Park, K. Y., An Extention of the Simple Mathematical Model by Gifford and Hanna for the Estimation of Urban Air Pollution, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tennessee, Contribution No. 60.

Plate, E. J., 1971: Aerodynamic Characteristics of Atmospheric Boundary Layers, available from NTIS, number TID-25465.

Ranzieri, A. J., 1971: Air Pollution and Roadway Location, Design and Operation, California Department of Highways, Materials and Research Division, June, 1971.

Roberts, J. J., J. E. Norco, A. S. Kennedy, E. J. Croke, A Model for Simulation of Air Pollution Transients, in Proceedings of the Second International Clean Air Congress, Academic Press, 1971, pp. 1161-1167.

Shieh, L. J., B. Davidson, J. P. Friend, 1970: A Model of Diffusion in Urban Atmospheres: SO_2 in Greater New York, in Proceedings of Symposium on Multiple-Source Urban Diffusion Models, Air Pollution Control Office Pub. No. AP-86, pp. 10-11.

Shieh, L. J., P. K. Halpern, B. A. Clemens, H. H. Wang, F. F. Abraham, 1971: A Multiple-Source Diffusion Model for New York City, in Proceedings of the Symposium on Air Pollution, Turbulence and Diffusion, December 7-10, 1971, pp. 108-115.

Sklarew, R. C., A. J. Fabrick, J. E. Prager, 1972: Mathematical Modelling of Photochemical Smog Using the Pick Method, Journal of the Air Pollution Control Association 22 (11), 865-869.

Sklarew, R. C., D. B. Turner, J. R. Zimmerman, 1972: Modeling Air Pollution Concentrations Near Highways, EPA Division of Meteorology, Research Triangle Park, N. C., November, 1972.

Slade, D. H. (ed.), 1968: Meteorology and Atomic Energy 1968, U. S. Atomic Energy Commission TID-24190.

Thyer, N., K. J. K. Buettner, 1962: Part A: On Valley and Mountain Winds III, Part B: Valley Wind Theory. Final Report AFCRL-62-1082.

Turner, D. B., 1969: Workbook of Atmospheric Dispersion Estimates, Public Health Service Publication No. 999-AP-26.

Wang, I. T., D. M. Rote, 1973: A Finite Line Source Dispersion Model for Mobile Source Air Pollution. Argonne National Laboratory Paper #75-135.

Wendell, R. E., J. E. Norco, K. G. Croke, 1973: Emission Prediction and Control Strategy: Evaluation of Pollution from Transportation Systems, Journal of the Air Pollution Control Association 23 (2), 91-97.

Wolsko, T. D., 1971: Environmental Impact of Transportation Systems: Preliminary Report. Argonne National Laboratory, Center for Environmental Studies, November, 1971.

Zimmerman, J. R., R. S. Thompson, 1973: A Simple Highway Air Pollution Model ("HIWAY"), Environmental Protection Agency, June, 1973.

7.0 ACKNOWLEDGEMENTS

The authors would like to express their thanks to Mrs. Naydene Maykut and Dr. John Thielke for their valuable suggestions and assistance in preparing this report and to the Staff of the Washington State Highway Department for their cooperation and support.

REPORT DISTRIBTUION LIST

For

"A Critical Review of Mathematical Diffusion Modelling Techniques for Predicting Air Quality with Relation to Motor Vehicle Transportation"

Agreement Y-1540

No. Copies	Name	Address
25	HIGHWAYS LIBRARY	Washington State Department of Highways Highway Administration Bldg. Olympia, Washington 98504
15	RESEARCH & SPECIAL ASSIGNMENTS DIVISION	Washington State Department of Highways Highway Administration Bldg. Room 1A17 Olympia, Washington 98504
10	ENVIRONMENTAL PLANNING DIVISION	Washington State Department of Highways Highway Administration Bldg. Olympia, Washington 98504