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A Review of Methods for Predicting Air Pollution Dispersion

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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PREFACE

The recent increased societal awareness of environmental pollution has led to increased scientific attention to the field of mathematical modeling of urban air pollution. This publication represents the results of an extensive survey of such modeling, and addresses itself to three main objectives

(1) To review the theory employed

(2) To review the applications of the theory

(3) To suggest improvements in the theory and its applications

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INTRODUCTION

Rationale for Developing Atmospheric Dispersion Models

This report is the result of a survey performed to identify problem areas in modeling air pollution dispersion and to summarize the current state of the art for these areas. Included are a summary of previous urban dispersion models, a review of the underlying concepts and assumptions, the techniques employed, and recommended research efforts which potentially can improve the ability to predict the dispersion of pollutants in the atmospheric boundary layer. Specific recommendations are made for utilizing these models to study the effects of pollutant contributions resulting from aircraft operations. Emphasis is on areas which are of direct concern to NASA or to which NASA's expertise could readily be applied.

Numerous documented incidents exist in which death or health impairment to large numbers of people have been attributed to atmospheric pollution. (See ref. 1.) Some of the more notable cases occurred in the Meuse Valley in Belgium in 1930 (60 deaths); Donora, Pennsylvania in 1948 (20 deaths); and London, England in 1952 (3500 to 4000 deaths). Despite such staggering statistics (particularly the London incident), widespread public concern with pollution problems has developed only during the past several years. Much of this concern to date has been expressed in the logical, but difficult, first step of adopting emission standards. However, these standards may be too restrictive or not restrictive enough. They may be economically self-defeating, and uniform application of the standards may be unwarranted. Clearly, many aspects of the problem require further study.

The air pollution cycle begins with the production of pollutants* by natural or anthropogenic sources. After emission, the pollutants are dispersed by atmospheric motion. Finally, the pollutants contact receptors (that is, people, vegetation, or materials) and are removed from the atmosphere. The cycle is symbolically depicted in figure 1. Legislation has been adopted in some instances to establish emission standards to limit pollutants and to establish air quality standards to protect receptors. The ultimate concern is, of course, the effects of the pollutants on the receptor. However, understanding the dispersion part of the cycle is vitally important if the pollutant distribution is to be accurately predicted for a given set of emission standards. In particular, one desires a mathematical urban dispersion model which can predict the dispersal of pollutants over some specified region. By definition such a model must

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*Pollutant, contaminant, and effluent are used interchangeably and synonymously to mean matter injected into the atmosphere.

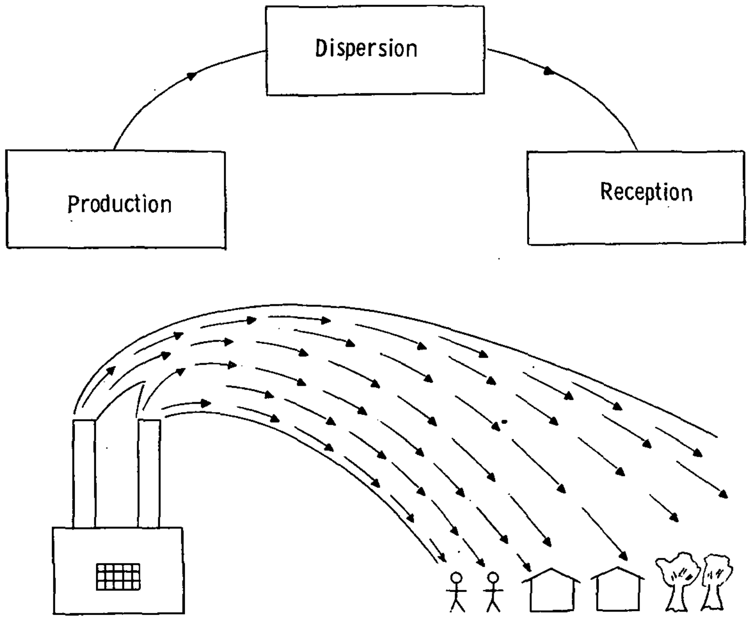

Figure 1.- Air pollution cycle.

include several components – an emission inventory, meteorological data, a diffusion submodel, and measurements for verification. A number of logical uses exist which justify construction of such models (ref. 2, p. 170). These uses include forecasting, planning, and supplementing measurements.

A reliable mathematical urban dispersion model would insure that emission standards and air quality standards are mutually consistent with one another. For example, conceivably the average concentration of a pollutant (if uniform mixing is assumed over an area) would be less than the level specified by air quality standards, whereas actual local concentrations at some points would exceed the specified levels. Thus, the model could determine whether air quality standards can be met, a set of emission standards being assumed. By carrying this idea one step further, the model could be used to identify adverse meteorological conditions that could create hazardous pollutant concentration levels. Alternate control strategies could then be devised and tested.

Possibly the greatest long-term benefits to be derived from dispersion models will be in the field of regional planning. For example, a reliable model would permit evaluation of the contribution of a proposed industry to the existing pollution profile of the region. Similarly, land usage strategies can be devised which will locate industry in a manner that will create minimal pollution levels for residential areas. Hindsight indicates that many problems could have been avoided by identifying an optimum location of an emissions source with the aid of a dispersion model.

Finally, dispersion models would supplement information from air quality monitoring networks. Because of high costs, relatively few monitoring stations are usually installed in a control region. Models could provide estimates of air quality in those areas where stations do not exist or are inoperative.

Thus, ample justification exists for developing mathematical models. Intelligent use of reliable models should lead to more effective and economical pollution control strategies. These strategies should be tailored to the case at hand while anticipating future requirements.

Classification of Models

Mathematical models can be described as empirical, theoretical, or semiempirical. Empirical models are generally derived by correlating extensive field data, whereas theoretical models are derived from fundamental principles governing the phenomena being considered. The most widely used models are semiempirical and are a combination of the other two methods.

Physical models simulate atmospheric motion with flow in a wind tunnel or water channel over a reduced-scale representation of the area being studied. They are particularly useful when it is impractical to develop a mathematical model. However, they may also be used to verify a mathematical model. Further comments in regard to wind tunnels and water channels are made in the appendix, but the primary emphasis herein is on mathematical models.

Models are further distinguished as being source-oriented or receptor-oriented. The source-oriented model determines pollutant concentrations at points removed from the source with known meteorological conditions and known source emissions. The receptor-oriented model determines the pollutant sources when meteorological conditions and pollutant concentrations at the receptor are known. Of course, in an area having many sources, a pollutant may easily lose its identity after mixing with others. In addition, the source of a pollutant presently being detected may no longer be upwind of the receptor because of the variation of the wind direction while the pollutant was traveling from source to receptor. Because of these difficulties, most models are source-oriented.

Urban models may be further classified according to assumptions concerning meteorological conditions. These classifications are climatological, steady-state, and transient models. Climatological models use weighted-average conditions that occur over long time periods such as a season. Steady-state models assume conditions to be constant over shorter time periods (for example, an hour to a day). Transient models allow meteorological conditions to change after short time periods on the order of 1 hour. These transient models use time-averaged conditions which are assumed to be constant over that time period.

In meteorology there are classifications based upon the scale, or the size, of the part of the atmosphere being considered in a given situation. The classifications have rather vague quantitative definitions and represent more of a qualitative distinction. Two of these classifications frequently used in connection with urban air pollution are microscale and mesoscale. The microscale refers to a part of the atmosphere which has a horizontal extent of up to about 6 km and a vertical extent from the surface up to 100 m or so. Thus, micrometeorology (the study of microscale phenomena in the atmosphere) is surface-dominated and includes the study of motion about a single structure (for example, building, tall smoke stack, or tower) or a cluster of structures. The mesoscale has a horizontal extent of 10 to 100 km. Mesometeorology includes the study of thunderstorms, urban area meteorology, and what are known as regional (that is, interurban) atmospheric phenomena.

Regardless of the classification, the previously mentioned components must be included to develop and use an urban air pollution dispersion model successfully. The following discussion illustrates the integral part each component serves in the complete model.

REQUISITES FOR DEVELOPING AND USING A DISPERSION MODEL

Emission Source Inventory

An inventory of all significant sources of pollution emission must of necessity be compiled for input for any dispersion model. The major pollutants of concern are carbon monoxide, oxides of sulfur, oxides of nitrogen, hydrocarbons, and particulates. Estimates of the total national emissions of these pollutants contributed by various sources are presented in table I (ref. 3). However, for mesoscale considerations, one

TABLE I. - UNITED STATES AIR POLLUTANT EMISSIONS IN MILLIONS OF TONS PER YEAR, 1969

Source	Pollutant emissions of –				
	Carbon monoxide	Sulfur oxides	Nitrogen oxides	Hydrocarbons	Particulates
Transportation	111.5	1.1	11.2	19.8	0.8
Fuel combustion in stationary sources	1.8	24.4	10.0	.9	7.2
Industrial processes	12.0	7.5	.2	4.8	14.4
Solid waste disposal	7.9	.2	.4	2.0	1.4
Miscellaneous	18.2	.2	2.0	9.2	11.4
Total.	151.4	33.4	23.8	36.7	35.2

of the less prevalent pollutants (for example, ammonia) may be of more importance than those pollutants listed in table I. Reference 4 gives a comprehensive discussion of additional pollutants and their respective sources.

A mathematical function must be constructed to represent each source. One must decide whether to represent the pollutants as emanating from point, line, or area sources. Much additional information concerning the details of the emissions must be included in a source model (ref. 5, p. 60).

For a stationary source the emission rates and their variation with time must be considered. For example, consider an electric power plant. The production of electricity and hence, the production of pollutant species vary with time of day, day of the week, or season of the year, depending on usage requirements. In most instances (for example, a tall power plant stack), some details concerning height of emission and effluent velocity are necessary.

For mobile sources further information is required. Traffic routes and density must be taken into account. Such factors as large variations in emission rates during the operational cycle must be considered. A typical case in point is the aircraft during idling, taxiing, taking-off, and cruising.

One must recognize the difficulty of obtaining accurate data to model certain sources. To treat a large number of individual home heating plants as an area source, for example, may require obtaining records of wholesale fuel sales, estimating rates of use by relying on past records of mean temperatures, and distributing the fuel usage according to population census data. Obtaining data to model a freeway as a line source is similarly difficult. For certain areas with active air pollution control programs, extensive emission data may be readily available. However, in some areas such information is virtually nonexistent and developing an emission inventory can be a formidable and expensive task.

Meteorological Data

All urban dispersion models require meteorological information as input data. The required data generally includes information on the wind, atmospheric stability, and mixing-layer depth. Panofsky gives an excellent introduction to air pollution meteorology in reference 6, and reference 7 gives an annotated bibliography for air pollution meteorology.

Knowledge of both vertical and horizontal components of wind velocity as a function of height and spatial position is desirable in the area being considered. Unfortunately, most wind data are obtained from a single official observation station at an airport or other site, which may be located some distance from the center of the model region. In this situation, one assumes that the data from the observation station are representative of conditions throughout the region. Furthermore, the vertical component of wind velocity is generally not measured. As a result of these difficulties, most models assume an average wind direction and speed that are everywhere constant. However, this assumption contradicts experience and may be one of the largest sources of error in the calculations.

The stability of the atmosphere is related to its ability to inhibit or enhance motion in the vertical direction. Stability is dependent on the gradient of the potential temperature* in the vertical direction. Measurements of vertical temperature profiles are often not available from meteorological stations. Pasquill (ref. 9, p. 209) has developed a method of estimating stability from surface conditions. This method can generally determine spread parameters necessary for the Gaussian plume method of analysis. (See ref. 10, p. 97.)

Most of the vertical mixing in the atmosphere occurs within several hundred meters of the ground. Vertical temperature profiles are required to determine the height of this "mixing layer." In the absence of local temperature measurements, great care should be used in estimating mixing-layer depth with data from remote stations. Local mixing-layer depth may be considerably different from that occurring at the remote station. For example, large heat inputs from urban areas may significantly increase the mixing-layer depth.

Diffusion Submodel

Atmospheric diffusion is the phenomenon occurring when particles, droplets, or gas molecules in the atmosphere separate from one another under the influence of turbulent eddies. The two mechanisms which form eddies are convective turbulence and mechanical turbulence. Convective turbulence occurs when heat causes the buoyant force exerted on the lower level of a fluid to be greater than that on the fluid above it. Mechanical turbulence results from the wind vector changing with height.

Ideally, one would determine the concentration of each species in a turbulent medium by solving the following turbulent diffusion equation (ref. 2, p. 176):

$$\frac{\partial \overline{c_i}}{\partial t} + \nabla \cdot \overline{u c_i} + \nabla \cdot \overline{u' c_i'} = D_{ij} \nabla^2 \overline{c_i} + R_i\left(\overline{c_1} + c_1', \ldots, \overline{c_n} + c_N'\right) \tag{1}$$

where

c_i concentration of species i per unit volume

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*Potential temperature is the temperature a parcel of dry air would have if brought adiabatically from its initial state to the arbitrarily selected standard pressure of 10^5 N/m^2 (10^6 dynes/cm^2). (See ref. 8.)

u	wind velocity vector
D_{ij}	molecular diffusivity
R_i	rate of production of species i by chemical reaction
t	time

The overbar indicates time-averaged quantities, unprimed quantities represent a mean value, and primed quantities represent a fluctuation from the mean value. The second and third terms on the left-hand side of equation (1) represent the advective* transport resulting from the mean wind and the diffusive transport caused by turbulent fluctuations in the wind, respectively. The first term on the right-hand side is the transport by molecular diffusion** and the second term is the chemical production. In general, equation (1) is a nonlinear partial differential equation that is intractable except by resorting to special numerical techniques of solution for such initial-value problems. Since the chemical production term is nonlinear except in special simplified cases, nearly all urban models to date have considered nonreacting species only; thus, equation (1) is linearized.

Even if chemical reactions are neglected, obtaining a solution to this equation is a formidable task. The difficulty arises from the lack of complete understanding of the physics of turbulence. In the past, two approaches to turbulence have been the gradient transport theory and the statistical theory. In the gradient transport theory, turbulent diffusion is assumed to be proportional to the local mean concentration gradient. The statistical theory studies the histories of the motion of individual fluid particles (that is, an ensemble of flows) and uses statistical parameters to represent the diffusion. The statistical theory of turbulence and of turbulent diffusion has resulted in a family of approaches which differ so greatly in sophistication and complexity that they appear to be entirely different and without a common origin (for example, see ref. 11, p. vi; ref. 12, pp. vii, 3 to 5; ref. 13, pp. 179 to 182; ref. 14, pp. 252 to 259; ref. 15; and ref. 16, pp. 119 to 121). An introduction to this increasingly important area may be gained from the following references: reference 17, pages 20 and 21; reference 18, pages 88 to 99; reference 10, pages 83 to 94; reference 19, pages 260 to 351; reference 20, pages 196 to 253; reference 21, page 370; and the references mentioned in the previous sentence.

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*Convection refers to the predominantly vertical, locally induced motions of the atmosphere; advection describes the predominantly horizontal, large-scale motions (ref. 8, p. 10).

**The turbulent diffusion is typically larger than the molecular diffusion by a factor of 10^4; thus, the molecular diffusion term is neglected.

The most widely used mathematical formula for describing turbulent diffusion in the atmosphere is the so-called Gaussian plume formula. This formula is a hybrid of the gradient transport theory and the statistical theory, since it is based upon the solution to a simplified form of the turbulent diffusion equation; and statistical properties of the atmosphere enter in the form of standard deviations. A Gaussian (also called bell-shaped or normal) distribution of species concentration seems to be reasonable since data show the distributions of velocity components to be nearly normal (ref. 6, p. 276). The velocity components are indicative of the air motion and, hence, of the diffusion of an effluent in the air.

A typical form of the Gaussian plume* formula for atmospheric diffusion is

$$c(x,y,z) = \frac{Q}{2\Pi\sigma_y\sigma_z\bar{u}} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\exp\left[-\frac{(z - H)^2}{2\sigma_z^2}\right] \tag{2}$$

where

x	horizontal distance from source in direction of wind vector and along the plume center line
y	horizontal distance perpendicular to and measured from the plume center line
z	vertical distance from ground to the plume center line
Q	mass rate of efflux of pollutant
σ_y	standard deviation in crosswind direction from the plume center line
σ_z	vertical standard deviation from the plume center line
$\bar{u}$	mean wind speed in x-direction
H	effective height of emission

The simplified turbulent diffusion equation assumes that the eddy diffusion coefficient for a given direction is constant. This assumption is obviously not true in the

*The term "plume" (also "cloud") is used to describe that part of the atmosphere where the pollutant emitted by a source appears to be concentrated. The visible edge of a diffusing plume is assumed to coincide with the point at which the pollutant concentration falls to 10 percent of its center-line concentration (ref. 10, p. 101).

atmosphere; thus, an empirical method has been developed that allows for the spatial variation of diffusion coefficients. This method expresses the concentration as a function of standard deviations, σ_y and σ_z, rather than of the diffusion coefficients. The standard deviations of the distribution of pollutant concentration in different directions are determined in various ways. The best method is the experimental determination of the standard deviations for a given area. However, when experimental data are not available, as is true in most cases, a number of alternate methods may be used. The most popular of these is the Pasquill-Gifford method (ref. 10, p. 101) which empirically fits a large collection of experimental data. Although the Gaussian formulas result from unrealistic assumptions, they have been successful in some applications because they are empirically fitted to atmospheric data (ref. 22, p. 112).

The effective height of emission H in equation (2) is the sum of the physical height of emission h_s (such as from a stack) and the plume rise Δh. (See fig. 2.) The plume rise is due to the initial upward velocity of the effluents as they leave a stack and to the buoyant force caused by the fact that the effluents generally are emitted with a temperature different from that of the ambient air. The plume rise may be negative in cases where the plume is more dense than the ambient air and consequently falls after leaving the source. These considerations illustrate the necessity of treating the plume as if it originates at some effective height rather than at the simple source height. The effective emission point is also assumed to be slightly upwind of the actual stack where the plume rises. Plume rise is beneficial in that the more a pollutant rises, the lower the pollutant

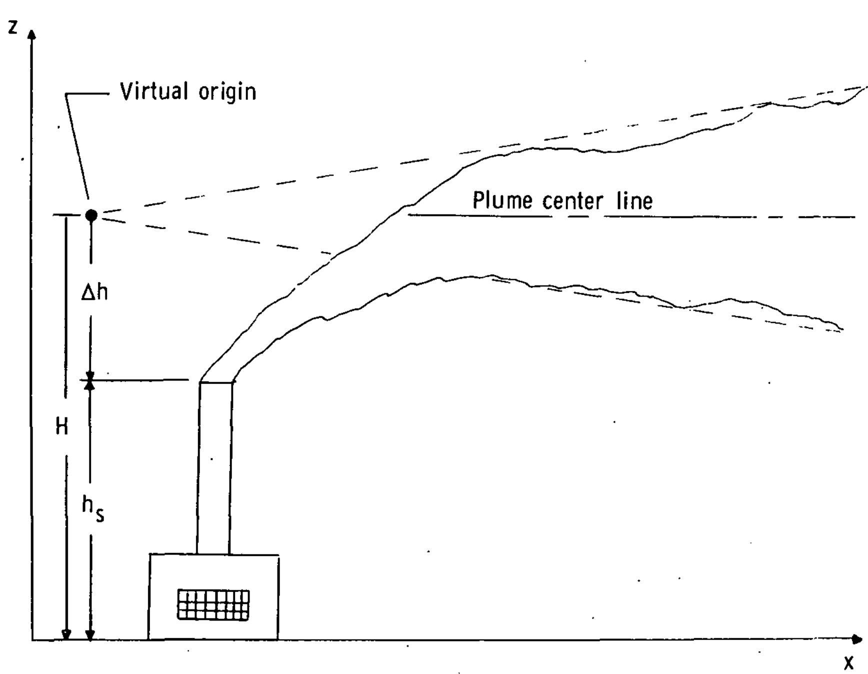

Figure 2.- Plume rise.

concentration is at the ground level. The plume rise phenomenon has received much attention in the last several years and a critical review of the subject is presented in reference 23.

Advective transport of pollutants is due to the mean wind speed $\bar{u}$. At the same time the effluent is being transported by the mean wind, it is being spread horizontally and vertically by atmospheric turbulence. This spreading is assumed to occur in such a way that the pollutant distributions are normal in the horizontal and vertical directions. The standard deviations of these two normal distributions are adjustable and increase with distance from a pollutant source. The horizontal spread is generally much greater than the vertical spread. In the Pasquill-Gifford method the horizontal and vertical standard deviations are graphically presented as functions of the distance from the source and of the atmospheric stability.

Most models assume that the mass of pollutants in the atmosphere remains constant; that is, no removal processes are occurring. This assumption requires diffusion formulas to account for plume reflection off surfaces or boundaries which the plume contacts. This assumption can readily be incorporated into the Gaussian distribution formula when the surface is the ground (ref. 16, p. 119) or an elevated inversion representing an impenetrable surface to the plume (ref. 24, p. 7). Gaussian plume formulas have also been modified to allow for removal of pollutants (ref. 25, p. 19).

Several simplified approaches which enable one to make pollutant dispersion calculations with a minimum of theoretical understanding (that is, a handbook approach) are given by references 24, 26, and 17. If a little probing into the theory is desired, references 21 and 10 are recommended. The most fundamental theoretical solution to the pollutant dispersion problem requires consideration of the set of governing partial differential equations, which are presented in chapter 1 of reference 27.

Measurements for Verification

A discussion of air pollution instrumentation and measurement techniques is beyond the scope of this paper. Interested persons are referred to reference 28, which presents the state of the art, current developments, basic and applied research needs, and an extensive bibliography in the field of pollutant measurement and monitoring instrumentation.

Several general comments are relevant concerning the role of measurements with respect to dispersion modeling. Because of the assumptions and uncertainties inherent in the source inventory, meteorology, and diffusion submodel, the predictions of the model must be validated by comparison with experimental field observations of air quality. To insure confidence in the model over a wide range of applicability, these observations must be carefully obtained over long periods from regions with varying characteristics of topography and meteorology.

REVIEW OF EXISTING MODELS

Some of the important mathematical models of urban air pollution have been summarized in references 2, 25, and 29 to 33. An excellent collection of some air pollution models and of recent thoughts on modeling is contained in reference 34. Other such collections which are more recent are references 35 to 38. The air pollution technical information center of the Environmental Protection Agency (EPA) at Research Triangle Park, N.C., provides computer searches which print out bibliographies (with abstracts) on selected subjects.* A review of several models which have received wide recognition and application follows in the chronological order of their publication.

Urban and Interurban Models

Frenkiel, 1955.- Frenkiel is considered to be the pioneer in mathematical modeling of urban air pollution for his analysis of atmospheric pollution in the Los Angeles basin as early as 1955 (refs. 39 to 41). The effluent from automobile traffic and incinerators in an area 6.4 km by 6.4 km (4 miles by 4 miles) square was assumed to emanate from a point at the center. The effluent emitted from a continuous point source during an hour was treated as a single puff. The dispersion of each puff was assumed to follow the binormal (Gaussian in the vertical and crosswind directions) distribution about the plume center line, the puff being transported by the mean wind which was allowed to vary with location and time. By superposing the concentrations arising from each major industrial point source and all the traffic and incinerator sources, estimates were made of the diurnal variation of pollutant concentrations at various locations in the Los Angeles basin. Frenkiel used an elementary Gaussian diffusion model with continuous point source emission rates and reflection of pollutants at the surface, and assumed that the ozone concentration was proportional to the product of concentrations of nitrogen dioxide and of hydrocarbons (ref. 40, p. 288).

Neiburger, 1959.- In 1959, Neiburger (ref. 42) noted the predominant meteorological influences (that is, light winds and a thermal inversion aloft) associated with the Los Angeles smog. Neiburger developed a model in which he assumed that an impenetrable inversion with a constant height of 400 m (a representative average height) was always present over Los Angeles. A further assumption was that the pollutants were vertically dispersed instantaneously and uniformly all the way up to the inversion lid. No horizontal

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*On March 31, 1972, the authors obtained a listing of more than 90 pages of such abstracts for the subject of mathematical modeling of urban air pollution since 1966.

turbulent diffusion was allowed and the horizontal spread was limited to that caused by the advective transport of the mean wind. Such a model can be used for predicting average concentrations for large regions. It cannot be used for small spatial scales because it does not include the complicated detailed meteorological conditions of an urban area.

Pooler, 1961.- In 1961, Pooler (ref. 43) developed a climatological model for sulfur dioxide pollution in Nashville, Tennessee. This model was based on more complete data than had been available for previous urban models. An inventory of the sulfur dioxide emission rates for each 1.6-km (1-mile) square area and an extensive number of sulfur dioxide measurements were obtained for the city of Nashville. Monthly wind roses* for the Nashville airport were utilized in the model. Source strengths were assumed to be constant for each month and the atmosphere was assumed to be neutrally stable. For the diffusion and transport, the pollutant from each source was assumed to be uniformly distributed in the horizontal direction over a $\pi/8$ sector downwind from the source. In the vertical direction the distribution was assumed to be Gaussian, the vertical standard deviation being dependent upon the wind speed. For each wind speed and direction the relative concentration at a point was determined by considering all surrounding area sources and by taking the weighted average contribution of these sources, wind frequency data being used as weights. This model was particularly useful for calculating the monthly mean concentrations.

Turner, 1964.- By use of the same data as Pooler, Turner (ref. 45) in 1964 introduced a daily operational model by devising a model for a shorter time period than Pooler. Turner made calculations for 2-hour intervals to show the diurnal variation and averaged 12 of these 2-hour intervals to give 24-hour values which yielded the day-to-day variations. The meteorological conditions used in the model were obtained by integrating over a 2-hour interval. The same meteorological conditions were assumed to apply over the entire city.

The dispersion and transport model differed from that employed by Pooler. Turner assumed the pollutant concentration to be binormal and attempted to modify the Pasquill-Gifford standard deviations to account for urban area effects. The area sources were treated as psuedo-point sources. The emissions from each 1.6-km (1-mile) square area were regarded as coming from a crosswind line source that corresponded to the plume of an upwind point source whose effective stack height was 20 m. The removal of SO_2 was accounted for by assuming that it decayed exponentially with a half-life of 4 hours. This half-life assumption limited the model to days when no precipitation occurred.

Miller and Holzworth, 1967.- In 1967 Miller and Holzworth (ref. 46) developed an urban model which treated diffusion in the mixing layer more realistically than had been

*A wind rose is a polar diagram which shows the frequency of occurrence of wind vectors at a given location (ref. 44, pp. 28ff.).

done by Neiburger (ref. 42). A major assumption of the model was that vertical diffusion followed the Gaussian distribution in the mixing layer until the plume intersected the top of the mixing layer (that is, the bottom of the inversion lid); this assumption is in contrast to the immediate vertical mixing and uniform distribution assumed by Neiburger. After intersection with the lid, the mass of the plume was assumed to be uniformly distributed throughout the mixing-layer depth. The Holzworth method was used for estimating the daily mixing-layer depths. (See ref. 47.) Another major assumption was the simplified treatment of sources. The sources were assumed to emit continuously at the surface (that is, effective emission height of zero) and to be uniformly distributed over the urban area. Then in a manner analogous to that used by Turner to handle area sources, the sources were regarded as a series of uniform, crosswind infinite line sources. The meteorological conditions and emission rates were assumed to be constant for intervals of 2 to 4 hours. These simplifications enabled users to perform the model calculations with a desk calculator instead of with a digital computer.

Basically, this dispersion model yields the average normalized concentration (that is, averaged by integrating over the entire city and normalized by dividing by the uniform line source strength). This concentration is dependent upon the wind speed, the size of the city, and the mixing-layer depth. The model is thus limited to estimating mean concentrations for entire urban areas and cannot predict pollutant concentrations on a small scale. Applications to Los Angeles, California, Nashville, Tennessee, and Washington, D.C., have yielded good results.

Hilst, 1967.- A group at the Travelers Research Center (now TRC, the Research Corporation of New England) has developed a receptor-oriented mesoscale air pollution model for the state of Connecticut (ref. 48). This model has become known as the TRC model or the Connecticut model. It predicts ground level concentrations of pollutants emitted from multiple sources. Spatially, the model considered a grid of 5600 area sources which were each 1.5 km by 1.5 km (5000 ft by 5000 ft), but included individual point sources for major industrial sources. The model gives the mean concentration averaged over a 2-hour interval for each grid area. The reason for this time scale is that although hourly emission rates of each source were part of the emission inventory, chronological variations in the wind field and in the atmospheric dispersion conditions were accounted for by input variables which were averaged over 2-hour intervals.

The pollutant concentration within the volume of air over a given grid square at a given time is determined by following the volume backward in time along its trajectory. The model computes the amount of material injected into the volume by the sources that can contribute along the trajectory. This computation is made by using the emission rate of the source during the time period that the volume of air was over that source. The large-scale wind fields which determine the trajectories are analytically represented by stream functions. As the pollutants move along their trajectories, diffusion from each area or point source was represented by the binormal distribution. However, within each volume the concentrations were assumed to be uniform; this assumption is consistent with the spatial resolution of the model. The standard deviations used in the model were empirical values based upon the atmospheric stability and the travel distance for the appropriate trajectory from a contributing source to the area of interest. The loss of a pollutant was accounted for by a simple exponential decay term. The model has been actively used and up-dated since first being reported in 1967. An extensive validation study of the model was reported in 1970. (See ref. 49.) A recent report on this regional model has been completed for the Environmental Protection Agency. (See ref. 50.) The model has also been adapted for urban scale use and applied to metropolitan Toronto. (See ref. 51.) The regional application of the model was for an area of 12 950 km^2 (5000 square miles) (that is, the state of Connecticut), whereas the urban application was for an area of 632 km^2 (240 square miles).

Croke et al., 1968. - The Argonne National Laboratory (ANL) began developing a computerized, transient, urban air pollution dispersion model in 1968. (See ref. 52.) The model was developed for operational use in an air resources management system and has been reported in various stages of evolution (refs. 53 to 57). The model describes transients such as morning transitions in atmospheric stability and variations in the mixing-layer height. The transients are based upon piecewise-constant quantities (for example, source emission rates, wind vectors, and atmospheric stability parameters). The fundamental time interval for the model is 1 hour, quantities being assumed constant for that period.

The diffusion and transport are determined from consideration of individual puffs of effluent instead of plumes. A puff or small cloud results from the instantaneous release of a discrete amount of effluent from point or area sources. The puffs are assumed to diffuse with a Gaussian distribution in three dimensions. The standard deviations for the three-dimensional Gaussian distributions were obtained from two sources of empirical curves, the Pasquill-Gifford curves (ref. 24, pp. 8 and 9) and Turner's curves (ref. 57, p. 25). The transport of the puffs is obtained from the piecewise-constant hourly wind vectors. The Gaussian puff formula is treated as a mathematical kernel. The concentration resulting from a continuous-source plume is then obtained by integrating over time with a convolution integral. Since all puff formulas must be integrated over time for continuous pollutant sources, this type of dispersion model is often referred to as an "integrated puff" model.

One of the advantages of using the integrated puff model is that it is possible to evaluate the effect of an area source on locations within the area as well as external to the area. Two important features of this particular model study, which was applied to

Chicago, are the ability to simulate near-zero wind speed conditions and the availability of a very large data base for validation studies. The Chicago telemetered air-monitoring network gave over 3 years of data consisting of 15-minute averages from 8 stations for SO_2 concentrations, wind speed, and wind direction. Also, the SO_2 hourly emission estimates were based on a 2-year inventory of SO_2 sources. The SO_2 concentration data were not used to adjust the calculated concentration to agree with the Chicago area measurements, but rather for validation studies. By not "tuning" the model to the data of a given area, its generality can be maintained.

This elaborate air pollution model is incorporated into an extensive master air pollution data management system. This system is employed to store, retrieve, process, analyze, and display emissions, meteorology, and air quality. The system can then be used to study meteorological dispersion, to form and input data arrays, and to validate its own theoretical predictions against recorded air quality data.

Lamb, 1968.- Most of the urban air pollution models reviewed thus far have assumed that the pollutants diffuse with a Gaussian concentration distribution. A more rigorous approach which attempts to solve the general diffusion equation was developed at the University of California at Los Angeles and reported by Lamb (ref. 58) in 1968. Neiburger also reported on this model in 1968. (See ref. 30.)

Although the approach is rigorous, it still involves a certain amount of empiricism in that the turbulent diffusion coefficients vary in such a way that experimental data are satisfied. Nevertheless, the model as reported in 1968 has been highly commended. In 1969, Seinfeld (ref. 2, p. 178) said that the model was ". . . the most extensive atmospheric diffusion model to date" and in 1970, Gifford and Hanna (ref. 59, p. 10), called it ". . . the most complete and flexible model we have examined." Actually, the model reported in 1968 represents but one stage in the development of a very general model.

As reported by Lamb and Neiburger (ref. 60), the intent is to construct a model for the general study of pollutants in an urban area satisfying the following stringent requirements:

(1) It must be able to deal with completely arbitrary distributions of sources with emission rates variable in space and time.

(2) It must permit an arbitrary distribution of initial concentration.

(3) It must permit the concentration and governing parameters to vary with time.

(4) It must allow variable diffusion coefficients.

(5) It must allow spatial and temporal variations of wind and temperature structure including variations of inversion height if an inversion serves as the upper surface of the model.

(6) Removal of the contaminants at the ground, variable with time and location, must be allowed for, as well as leakage at the upper surface of the model (for example, the inversion base).

(7) The chemical and photochemical reactions of the pollutant in question with other constituents of the air and with sunlight must be taken into account.

The model development is broken up into two phases. The first phase deals with the first six requirements (that is, the nonchemical aspects). The entire second phase will be devoted to pollutant chemistry. The model described in reference 60 satisfies requirements (1) to (4), and others are partially satisfied. The partially satisfied requirements are as follows:

(1) The winds are allowed to vary with time and in the horizontal direction, but are assumed to be constant in the vertical direction.

(2) The upper surface of the model is assumed to be an inversion at a constant height.

(3) The adsorption of the contaminant at the ground is assumed to be a fraction of the local concentration and is constant in time and in space.

(4) The decay or the production of the contaminant is represented by a time-varying term.

This model represents a new generation in the mathematical modeling of urban air pollution.

Shieh et al., 1969.- A few months before the Argonne National Laboratory (ANL) began work on their mathematical model, a group at New York University (NYU) independently began work on a model using a very similar approach. The NYU model was a very sophisticated source-oriented model based upon the three-dimensional Gaussian puff diffusion assumption with piecewise-constant input quantities and required a digital computer for solution. It could handle transients, consider different-size source areas, and had a very large data base. However, the model was oriented to the New York City area and thus is not as general as the ANL model. For example, the ANL model evaluated standard deviations of the diffusing Gaussian puff by means of widely used empirical curves, whereas the NYU model used empirical formulas whose parameters were evaluated by using New York City data.

The model was reported at the Symposium on Multiple-Source Urban Diffusion Models (ref. 61), and the final report was made in December 1969 (ref. 62). Apparently, the NYU model has not been as actively refined as the ANL model has.

Eschenroeder and Martinez, 1969.- Eschenroeder and Martinez (ref. 63) have developed an urban model for the Los Angeles basin. It is the only model which incorporates chemical reactions in an operational sense. The model is based on the species continuity equation (that is, the diffusion equation). Photochemical reactions are accounted for by the "lumped parameter" approach, which reduces 17 or more reaction steps to seven.

Horizontal advection of the pollutants by the mean wind is considered, but crosswind diffusion is neglected because of the nearly uniform distribution of emission sources. The model allows vertical diffusion with the vertical eddy diffusion coefficient as a prescribed function of height. Mean vertical convection is neglected because it is suppressed by the stable Los Angeles atmosphere.

The chemical reaction rate coefficients were obtained either from the literature or by adjusting to approximate laboratory results. By using finite rate chemistry, the model calculated concentrations of seven species found in the Los Angeles basin. Realistic concentrations could then be found by adjusting the reaction coefficients.

Eschenroeder and Martinez are continuing to work on the model by maintaining the somewhat simple dispersion assumptions but considering increasingly complex chemical reactions (ref. 64 and ref. 32, p. 2.17).

Highway and Airport Models

Models for highway and airport air pollution are in many ways similar to urban models. The highways are treated as a succession of straight-line sources, and airport runways and taxiways are treated as line sources. These mobile sources emit their pollutants horizontally as opposed to the vertically directed effluents from stationary sources. However, highway and airport models have received attention only in the last several years as compared with the 15 years that urban models have been in existence.

On a total mass basis, transportation is the source of more than half of the pollutants arising from anthropogenic activities. (See ref. 3.) The automobile is the primary source of these pollutants and is widely recognized as the main contributor to urban air pollution. Although aircraft account for less than 2 percent of the total pollutant mass, in the vicinity of airports the resulting emission concentrations are of the same level as concentrations in urban areas. This fact, coupled with the projection that aircraft activity will increase at the rate of 10 percent per year over the next decade (ref. 65, p. 3), requires that an assessment be made of the pollutant burden on the community surrounding an airport.

Highway and airport models are not as refined as urban models. Source inventories are not well developed nor is the best way to go about developing these inventories agreed upon. Most vehicular air pollution and a substantial part of airport air pollution come from sources at the ground level where the typical Gaussian treatment is more dubious than for emissions from stacks. Chen and March (ref. 66, p. 10) have accounted for this fact by using generalized eddy diffusion coefficients instead of assuming a Gaussian distribution of pollutant concentration. Highway air pollution modeling is discussed in references 66 to 68. Airport modeling has been treated in references 69 to 71.

LIMITATIONS OF PRESENT MODELS

The criteria for judging the performance of a mathematical urban model are somewhat vague and arbitrary. In the present state of the art relatively crude agreement between predictions and measurements can be expected. For example, Bowne et al. (ref. 51, p. 19) indicate that 60 percent of the model predictions for metropolitan Toronto are within a factor of two of the corresponding measurements. Lamb (ref. 58, p. 75) presents table II of 18-hour averages of carbon monoxide concentrations at 12 stations in the Los Angeles area. Only seven of these 12 predictions (approximately 58 percent) are within a factor of two of measured values. As a final example, figure 3 (ref. 62, p. 78)

TABLE II. - CARBON MONOXIDE CONCENTRATIONS

IN LOS ANGELES

Station	Observed 18-hour average, ppm	Computer 18-hour average, ppm
Downtown	16	22
Azusa	13	3
Pasadena	17	15
Burbank	16	7
East Los Angeles	12	5
West Los Angeles	16	13
Long Beach	14	8
Hollywood	17	7
Pomona	13	3
Lennox	13	11
Anaheim	9	7
La Habra	6	3

illustrates large scatter between observed and predicted values of SO_2 concentrations for various stations over Manhattan Island. Model performance and accuracy are discussed by Mahoney (ref. 5, p. 47), Moses (ref. 25, p. 26), and Pasquill (ref. 21, p. 387). Accuracy expectations of these kinds can be explained by examining the limitations and deficiencies of existing models.

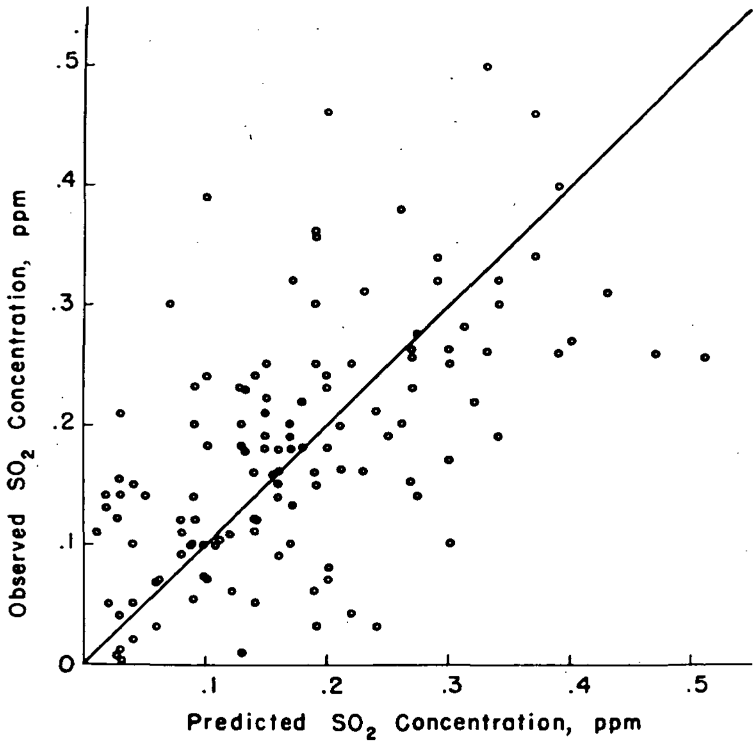

Figure 3.- Scatter diagram of variation of observed SO_2 concentration with predicted SO_2 concentration. (From fig. 35, ref. 62.)

Atmospheric Transfer Mechanisms

Turbulent diffusion theory.- The first and most fundamental deficiency in mathematical modeling is in the theory of atmospheric turbulent diffusion. Mahoney (ref. 5, p. 71) comments: "Because air pollution models must attempt to describe turbulent dispersion processes in the atmosphere, the models cannot be expected to meet very restrictive accuracy limits." Theories describing turbulent atmospheric processes are in need of fundamental advancement. An integral part of the problem is understanding the phenomenon of turbulence itself. In fact, the most serious defect in the recent direct approaches to equation (1) is the lack of a good theory relating mass fluxes to meteorological parameters and pollutant concentration gradients (that is, the lack of a good constitutive theory (ref. 22, p. 114)). Currently, these models use the gradient transport theory.

Two theoretical approaches to obtaining a more fundamental understanding of turbulent diffusion are generalized eddy transport models and stochastic modeling.

Typical of the generalized eddy transport technique is the method of "invariant modeling" of Donaldson (refs. 72 to 74) and the work done at Los Alamos Scientific Laboratory (refs. 75 to 77). Essentially these approaches involve writing an equation containing triple-velocity correlations for the double-velocity correlation terms (for example, the Reynolds stresses). Thus, one models the triple-velocity correlations rather than the double-velocity correlations. One advantage of such an approach is that heat can be transferred in the direction of increasing temperature (that is, a counter gradient flux) such as may occur near the top of the planetary boundary layer.

Stochastic representations of turbulent diffusion have been achieved by using a stochastic continuity equation as done by Lamb (ref. 32, p. 2.16; and ref. 78) or the analogy to the Langevin theory of Brownian motion (refs. 79 to 83). In the Langevin analogy the acceleration process moving two particles apart (that is, diffusing them) is assumed to have an infinitesimal duration (ref. 81, p. 1109). The Langevin type equations have been used to study the dispersion of material such as particles and aerosols which have finite size and mass but do not necessarily follow the motion of fluid parcels. Peskin (ref. 81, p. 1111) indicates that much additional work needs to be done in the way of refining the Langevin equation model.

Stochastic modeling leads to a confrontation with one of the most fundamental unsolved problems in the study of turbulent diffusion – the relationship between Lagrangian (moving parcels) and Eulerian (fixed point) quantities. This problem has been treated by Lumley (ref. 84) and Corrsin (ref. 85). An article by Corrsin on the Eulerian and Lagrangian theoretical approaches to turbulent diffusivity is given in reference 86. Peskin (ref. 81, p. 1109) and Sklarew (ref. 87, pp. 12ff.) give brief introductions to the problem.

Another area where the relationship between Eulerian and Lagrangian quantities arises is in the use of wind-fluctuation data. The operational air pollution models based on the Gaussian plume formulation greatly benefit from using actual wind fluctuation data for a given locality (ref. 88, p. 1068). However, these measurements are Eulerian quantities, whereas the theoretical formulations are in terms of Lagrangian quantities (ref. 81, p. 1109).

Diffusion coefficient representation. - Current operational models are limited because the diffusion coefficients cannot be specified as functions of spatial coordinates in terms of the various atmospheric stabilities and, to a lesser extent, of the surface roughness.

No urban atmosphere is uniform in a horizontal plane nor is the urban surface uniform. Although most models allow diffusion coefficients to vary with the horizontal downstream distance, none allow the coefficients to vary with horizontal crosswind distance from the plume center line.

An urban atmosphere is not uniform in the vertical direction, yet most models assume that parameters do not vary with altitude. In a study by Mahoney and Egan (ref. 89), ground level concentrations were found to be controlled significantly by the variability of the vertical diffusion coefficient with altitude. The study further reveals that the rate of removal of pollutants depends upon the details of the vertical distributions of the wind speed and of the vertical diffusion parameter in the mixing layer. Pasquill and Smith (ref. 88, p. 1068) have emphasized that the failure of the Pasquill-Gifford standard deviation curves to distinguish between elevated and ground sources leads to errors. Systematic changes occur with altitude in the natural dispersive action of the atmosphere with the likelihood of encountering sharp discontinuities in the flow structure as one goes higher. Thus, the neglect of vertical variations is a severe limitation.

A need exists for more detailed study into the effect of stability on plume spread. Also, a more fundamental basis for the classification of stability conditions is needed (ref. 88, p. 1071) in lieu of the simple Pasquill technique mentioned previously. Davidson (ref. 90, p. 156) suggested that multiple inversion layers are present over some urban regions and these layers will have to be considered.

Models need to be extended to account for the effect of surface irregularities on dispersion. The Pasquill-Gifford dispersion curves are valid only for level, uniform terrain, which is much more ideal than occurs in areas where air pollution is a concern. The roughness can be implicitly accounted for by using on-site turbulence data, but these data are usually unavailable. Thus, most models omit the effect of surface roughness, which can be in the form of large-scale features or a number of small-scale features, man-made or naturally occurring (ref. 5, p. 65). None of the several theoretical treatments of boundary-layer adjustment offer a satisfactory practical method which accounts for the progressive adjustment of dispersive properties to the everchanging surface (ref. 88, p. 1070). Pasquill and Smith (ref. 88) feel that it is now possible to make a reasonable allowance for the effect of the general degree of roughness on vertical dispersion.

Interurban scale modeling. - An increasingly important need is the requirement for mathematically modeling the behavior of pollutants as they travel from one city to another. This requirement has been brought about by the consideration of planning activities to control air pollution in highly industrialized urban corridors (for example, the Boston, Massachusetts, to Washington, D.C., corridor in the Northeastern United States). An urban model for a city in such a region is rather meaningless without including the pollutant influx from surrounding cities, as attested by the difficulties reported in reference 91. Dispersion models for such large regions ($\approx$100 km) should include the details of atmospheric stability profiles, which are important in the long-distance transport of pollutants. The vertical spread of plumes transported for times of several hours or more may be much less than a Gaussian model would indicate (ref. 5, p. 75). Rather, the pollutants may reside in a relatively small, stable vertical layer over long distances.

Pasquill and Smith (ref. 88, p. 1071) feel that for diffusion over long distances, the least one can do in the way of mathematical schemes that adequately reflect the broad physics of a real diffusion process is to solve the parabolic diffusion equation with both the wind speed and the diffusion coefficients given as functions of height. One of the major problems in such a solution is properly specifying the diffusivity profile in relation to the meteorological conditions (ref. 21, p. 388).

Atmospheric interfaces.- Mathematical models for the turbulent fluxes of mass (that is, water vapor), momentum, and heat at atmospheric interfaces and within the surface boundary layer (up to 100 m above the surface) are in a poor state of theoretical development and in need of more explicit treatment (ref. 89, p. 1157; and ref. 92).

In the vicinity of lake and ocean shores, an interaction occurs between the mass of air which is influenced by the body of water and the mass of air influenced by the land. Also, interfaces exist between the air and the land and between the air and the body of water. At all these interfaces one is faced with basically the same phenomena – sudden changes in the transport properties and the attendant atmospheric transport mechanisms for mass, momentum, and heat. Several experimental studies (for example, refs. 93 and 94) have been directed toward lake effects on atmospheric dispersion. Such studies could serve as springboards for theoretical advancements.

Turbulent energy and diffusion are intimately connected in the atmosphere. Therefore, knowledge of how the energy is transferred from motion of one scale to motion of another scale is important. Such energy exchanges between air masses of different characteristic scales are poorly understood. Synoptic scale (ref. 44, p. 19; synoptic- or cyclonic-scale phenomena have a horizontal extent of 100 to 1000 km) forecasts about large frontal systems cannot presently be related to the urban scale mesometeorological phenomena (ref. 89, p. 1152). The manner in which the energy input from a passing front affects turbulent diffusion on an urban scale is not known. Similarly, the effect of an urban heat island on stability characteristics in the planetary boundary layer has been studied by Olfe and Lee (ref. 95), but the phenomenon is not fully understood. Finally, one needs to predict how local circulations can be formed by tall structures and how the circulations affect ground-level pollutant concentrations. This last problem is an example of a mesoscale to microscale interaction.

Removal and Transformation Processes

Many important physical phenomena besides atmospheric turbulent dispersion are not satisfactorily included – if included at all – in current models. Two of these phenomena are removal and transformation processes. These phenomena are thought to be the most important causes of uncertainty for models dealing with long residence times for pollutants (for example, models for an interurban scale where hours are required for pollutants to be transported from one city to another, or models that use quantities which are obtained by averaging over a time period of hours). Even with advances in turbulent dispersion theory, the present lack of knowledge about the removal and transformation of pollutants in the atmosphere would severely limit models (ref. 5, p. v).

The assumption is usually made that the loss rate for a pollutant is directly proportional to the amount of pollutant present (ref. 25, p. 19). This assumption results in an exponential decay factor which contains a loss parameter (also called a loss constant or time constant). This loss parameter is a function of chemical species, the relative concentrations of the species, meteorological conditions (that is, local wind fields, ambient temperature, incoming solar radiation, and water vapor present), and topography. The loss parameters are determined from experimental data. However, experiments of this kind are very difficult to perform; consequently, only limited data are available. The result of having only limited data is that the loss parameters in use are crude approximations to reality, and much more research into the adsorption rates of pollutants onto surfaces is necessary. The different adsorption surfaces studied could be as general as urban, rural, and water or as specific as vegetation, pavement, wood buildings, masonry buildings, metallic buildings, level grasslands, and rolling woodlands. The mechanisms which cause adsorption are gravitational settling, diffusion down to and impacting with the surface, and precipitation scavenging (ref. 29, pp. 211 to 215; refs. 96 and 97; and ref. 98, pp. 179 to 183). No model studies have yet incorporated the details of these mechanisms (ref. 5, p. 73).

A large area for further research is physical and chemical transformations.* Aerosol** formation is an important, but poorly defined, physical phenomenon which causes an extinction of ultraviolet radiation and a visibility reduction. These effects have not been explicitly treated in models as yet, but eventually should be. The role of aerosols in atmospheric chemical reactions is unknown quantitatively. In fact, the whole area of heterogeneous chemical reactions on either particulate surfaces in an aerosol or urban surfaces remains obscure (ref. 63, p. 10).

In source-oriented models the pollutant concentration at a given receptor is obtained by taking the linear sum of the concentrations due to each source. However, in models treating chemical reactions, the rate of production of a species is a nonlinear function of the concentrations; thus, the rate of production in the overlapping region where two chemically reacting plumes intersect is not simply the sum of the rates in the individual plumes. Neiburger and Chin (ref. 32, p. 2.17) suggest that before these nonlinear chem-

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*Reference 99 gives a comprehensive assessment of the state of knowledge in atmospheric chemistry.

**An aerosol (ref. 100, p. 231) is a system with either a solid or a liquid dispersed in a gas (for example, cigarette smoke is an aerosol of solid ash dispersed in air).

ical reactions can be incorporated into models, better methods must be developed for integrating equation (1), for the case of transport and diffusion, within an Eulerian framework. When these models become available, an efficient method will be required for solving systems of equations which represent the simultaneous interaction of many reacting species as they are transported and diffused.

Along with the aforementioned needs, an even more basic and pressing need is the determination of which reactions are significant and their reaction rate coefficients. Chamber experiments are felt to be essential in the determination of the significant reactions and their rate coefficients. Specifically, Eschenroeder and Martinez (ref. 63, p. 9) state that chambers should be used to study the interactions in hydrocarbon mixtures which have widely differing reactivities. Reference 63 also states that experiments are needed to determine the distribution of nitrate compounds in polluted air so that the nitrogen balance may be solved.

Another research need is the study of mixedness* and its influence on chemical kinetics in reacting flows (ref. 63, p. 10; and ref. 101, p. B-9). This problem area has recently been raised and is felt to be of fundamental importance; thus, it may eventually need to be put into a practically applicable technique. Unfortunately, chambers are not suited to experimental studies of this problem because they do not permit proper simulation of flow-field turbulence.

Photochemical smog formation has long been recognized as important in urban environments, and as early as 1956, Frenkiel (ref. 40, p. 287) developed a simple, nonlinear model to examine the daily variability of ozone (a smog constituent) in the Los Angeles basin.** However, as yet the details and rates for the various reactions involved in smog formation have not been incorporated into urban dispersion models (ref. 5, p. 73).

Data Base

As mentioned earlier, the most widely used mathematical models are semiempirical. This situation is due to the lack of a completely theoretical way to describe the diffusion of atmospheric pollutants. With semiempirical methods, experimental data are necessary for the evaluation of parameters if one wants to get accurate results. As one might expect, complete input – or "external" – data (meteorological conditions, emissions, background levels of pollutants, and so forth) are not available on a routine basis for any sizable urban areas. Singer and Freudenthal (ref. 102, p. 545) feel that the limitations of present urban and regional models are due more to an inadequate data base than to inadequate physics.

*Mixedness refers to the spatial uniformity of reactions and homogeneity of the reactants and the products.

**Seinfeld gives an introduction to photochemistry and its inclusion in dispersion modeling in reference 2.

The available data used for initial conditions, boundary conditions, source strength histories, and so forth, are subject to significant uncertainty. This uncertainty is especially true for pollutant concentration data, because they are influenced by an unorganized pattern of local emission sources in most urban areas (ref. 89, p. 1157). The initial and boundary conditions are important if one attempts the numerical solution of the diffusion equation. Also, for any mathematical model, the smaller the area covered, the more sensitive the results are to errors in the specification of initial data fields. Larger scale models are more coarse and tend to smear out small errors.

The points mentioned in the preceding paragraphs lead one to the conclusion that a deficiency of detailed urban models is that they exceed their data base. In other words, the limited amount of data used as input to these models frequently limits them to predicting gross effects and trends. The more detailed the model, the more detailed the input data need to be.

The nearly unlimited need for all kinds of data is illustrated by a recommendation in reference 103 that field measurement programs are needed for observing the processes of chemical reactions, phase changes, deposition, and atmospheric transport and diffusion. Some of the specific data deficiencies will now be examined.

All current air pollution models require forecast meteorological data from "external" sources (for example, the local National Weather Service Office). Therefore, the accuracy of the air quality forecast by a model is limited by the accuracy of the forecast meteorological data which is often the greatest source of uncertainty for model predictions. Another aspect of Weather Service data that can make it inapplicable to urban models is that it reflects average conditions at rural or, at best, suburban locations (that is, airports where Weather Service observing stations are located) rather than urban conditions. Ultimately, one can expect the development of urban models that contain methods of meteorological forecasting.

Data on the properties of turbulence over urban areas are scarce. If the governing partial differential equations are being solved, data of this type are necessary to represent the diffusion coefficients which appear in the equations. If the operational procedure using Gaussian distributions is being used, these data would permit the development of standard deviation curves which would be the urban counterpart of the Pasquill-Gifford curves. As mentioned previously, the rate of removal of pollutants is strongly dependent upon the details of the vertical distribution of the diffusion parameters. (See ref. 89.) Therefore, even if the data are available for urban standard deviation curves of σ_y and σ_z, one cannot expect accuracy on the smaller scales until the vertical distributions (that is, $\sigma_y(z)$ and $\sigma_z(z)$) are also known. Reference 88 points out that if urban turbulence data are available, one must be aware that the turbulence data have a complex dependence on sampling time. In other words, data used to obtain σ_y (which determines the plume width) and σ_z (which determines the plume depth) are affected by the sampling time used in collecting the data. The dependence is not understood fully and is an area requiring research.

Another factor that limits the accuracy of most mathematical models is that they use constant wind speed and direction data for entire urban areas. Wind data are usually obtained from nonurban monitoring stations, as just mentioned. Thus, there is a requirement for more detailed wind field data. This need exists at the mesoscale which includes the urban scale and the interurban scale. On the interurban scale Hilst (ref. 49) has found the Connecticut model calculations to be very sensitive to inaccuracies in the wind-direction specification. The conclusion is that in models where the pollutant transport is for distances as great as 20 km, the accuracy will normally be limited by the lack of detailed wind field data on such scales. On the urban scale the results are dependent not only upon the wind variation in the horizontal direction but also on the variation of the wind in the vertical direction. By referring to the results of reference 68, the details of the vertical distribution of the velocity vector are seen to have an important influence upon the rate of removal of pollutants. Furthermore, observations of the vertical component of the velocity vector are not made routinely. Therefore, much more extensive specification of the mean wind field in urban areas is necessary. Pasquill has reviewed the general state of knowledge about the wind characteristics near the ground in reference 104.

Removal and transformation processes have already been mentioned as deficiencies in urban modeling; consequently, one should not be surprised that there is a deficiency of data for these processes also. Mahoney (ref. 5, pp. 72 and 73) points out that experiments to evaluate atmospheric transformation parameters are very difficult because atmospheric dispersion is dominant during the first few minutes after the discharge of the effluent. This initial dispersion usually reduces concentrations by several orders of magnitude and masks the influences of transformation processes. For this reason, frequent sensitivity and calibration checks on available monitoring instrumentation are required if the desired information is not to be lost in instrument errors. Therefore, the prospect of obtaining adequate and reliable data for these processes is dim for the near future and represents an area for much study. In order to supply the required data, the National Research Council (ref. 103, p. 39) recommends regional scale (≈100 km) measurements, for several areas and time periods, of (1) the chemical composition of precipitation and (2) the dry fallout (deposition) rate. Therefore, the necessary instrumentation and measurement techniques for obtaining data on removal and transformation processes must be developed.

In addition to the lack of understanding about aerosol formation, there is a deficiency of data for some aerosol properties. In particular, the lack of data for urban aerosol radiation absorption and scattering coefficients precludes accurate calculations. Atwater (refs. 105 and 106) has shown that atmospheric radiation influences the urban temperature profile and that the radiative temperature changes are significantly affected by the aerosol concentrations present.

A few more miscellaneous deficiencies in the data base are worthy of mention. Roberts et al. (ref. 57, p. 27) state that the trajectory of the center line of a plume can rarely be specified to better than $\pm 10^{\circ}$; therefore, short-term estimated and observed concentrations can easily differ by a factor of two, regardless of the model employed. Chen and March (ref. 66, p. 40) suggest field measurements of highway-associated air pollution, because no data could be found for comparison with their analytical model calculations. Finally, up-to-date and accurate inventories of emissions from all sources in a region of interest are always desirable, as previously mentioned in the section "Emission Source Inventory."

Gifford and Hanna (ref. 59, p. 1148) point out that no complete set of urban air pollution data is accepted as definitive for the purpose of trying out diffusion models to determine their accuracy. A completely defined problem (that is, initial conditions, boundary conditions, time and space histories for source emissions, meteorological parameters, and concentration measurements) is needed so that the calculated solution can be validated for any model. As more general models (that is, models not limited to applications at only one site) are developed, such a complete set of data will be increasingly useful.

The fact that the data base is not adequate for detailed mathematical models is not an altogether bad situation, because models frequently identify data requirements. Neiburger and Chin (ref. 32, p. 2.17) suggest that the sensitivity of models to the various types of data will enable one to determine the adequacy of available measurements. As an example, reference 89 identifies the importance of the details of the vertical distributions for the wind and the diffusion parameter. Similarly, in reference 49 the wind direction is seen to have a strong influence on accuracy. Obviously then, models can be an aid in designing field experiments and in establishing monitoring stations.

Solution Procedures

In those urban models employing computerized numerical techniques in the solution procedure, one is confronted with the problem of obtaining an accurate calculation within the bounds of reasonable computer time and storage. The following references cite examples of this problem.

Peskin (ref. 81, p. 1114) alludes to some of the difficulties encountered in developing two- and three-dimensional numerical solutions for turbulent diffusion problems. For example, a grid size that is small enough to detect sufficiently small initial separations of diffusing particles requires very long computer times.

Similarly, Seinfeld (ref. 2, p. 192) mentions that in order to include satisfactorily the assumption of instantaneous, uniform mixing of effluents, an air quality region must be represented by small mixing cells. However, when one uses a large number of small cells for accurate atmospheric representation, large computing times are encountered. Thus, as is true for all numerical solutions, the computerized urban models trade accuracy for reduced computational time.

Egan and Mahoney (ref. 107, p. 1) state that the use of virtual upwind point sources to represent emissions from area sources can lead to large errors in the calculations for several area widths downwind. Thus, treating area sources directly is desirable in urban dispersion models. Also, reference 107 illustrates that care must be used in the differencing method selected. For example, Egan and Mahoney (ref. 107, p. 2) found the accuracy of the advective term $u \frac{\partial c}{\partial x}$ in the diffusion equation to be particularly sensitive to the differencing approximation. Another caution to those working with differencing schemes is that one must frequently check the solutions to insure the conservation of mass and kinetic energy.

RECOMMENDATIONS AND CONCLUDING REMARKS

A consistent philosophy emerges from the foregoing review of previous urban air pollution models. All the reviewed models developed a solution by assuming the effluent dispersed according to a Gaussian distribution or, alternatively, by solving some form of the diffusion equation. Numerous important effects were neglected, as pointed out in the section describing model deficiencies. These models were formulated for application to a specific area and will not work well for an area different from that for which they were designed. Clearly, many aspects of urban modeling have been neglected and extensive research efforts, such as the EPA Regional Air Pollution Study at St. Louis (ref. 108), are needed.* However, the recommendations which follow are directed only to those aspects of modeling which promise to improve modeling capabilities significantly in the near future and to enable the utilization of the models in determining pollutant contributions. The recommendations are as follows:

(1) An extensive network of measurement sites should be established in the air quality control regions designated by the Clean Air Act of 1967 to collect, on a regular basis, adequate meteorological and air quality data. The current dependence on data collected from stations remote from the region being modeled is one of the largest possible sources of error in present models, as was previously pointed out (ref. 5, p. 71).

*Many of the references cited in the present report contain recommendations dealing with the topic treated by the particular reference (for example, ref. 98) and reference 109 contains a lengthy list of research needs for the entire field of air pollution.

(2) Techniques should be developed to measure turbulence properties as a function of height over urban regions so that diffusion coefficients can be evaluated for use in computations.

(3) Reaction rates for postulated photochemical reactions should be measured in controlled laboratory experiments with particular emphasis devoted to reactions involving the highly reactive olefinic compounds (ref. 99, p. 6.1).

(4) A dispersion model should be developed based upon an initial value integration of the equations (that is, the time-dependent continuity, momentum, and energy equations (ref. 110, pp. 59ff.) coupled with the diffusion equation (ref. 2, p. 176)) which govern turbulent atmospheric motion in the earth's surface layer. In this type of analysis, the wind and temperature fields would be calculated concurrently with the pollutant concentrations.

(5) Functional representations which can correctly represent time-varying emission rates should be constructed for all types of pollution sources and should be incorporated into the dispersion model.

(6) The influence of topography upon the meteorological field should be included in the dispersion model. Obviously, very complex topographical features cannot be successfully modeled mathematically and can best be studied in the wind tunnel or water channel. However, flows with such features as mountains or valleys present could be studied by representing these features with simple geometric shapes. The effects of discontinuities in surface temperature at land-water interfaces and of varying surface roughness are also amenable to mathematical analysis.

(7) The transformation of constituent species of the flow by chemical processes should be included in the dispersion model with a set of kinetic rate mechanisms to represent the postulated reactions taking place. Although uncertainty exists as to the complete reaction mechanism, particularly in the instance of photochemical smog (ref. 2, p. 184), failure to include chemical transformations severely compromises the validity and usefulness of the model. Prior analyses have neglected the fluctuating part of the species concentration in the chemical production term of the turbulent diffusion equation. An in-depth analysis should be initiated to determine whether this approximation is indeed a good one. At present, the authors are unaware of any evidence to substantiate this approximation.

(8) Removal or "scavenging" processes, such as surface adsorption and precipitation washout, should be studied in a more fundamental way and included in the dispersion model. At present, the rates at which these processes occur and the variables on which they depend are unknown.

(9) After development of the dispersion model including the effects of topography, chemical transformations, and removal processes, the model should be validated by

comparing calculated results with experimental field observations. The model should be validated for areas having widely differing characteristics of topography and meteorology to insure its general applicability.

(10) An inventory of all sources of pollution at an airport must be determined. This inventory should include, but not be limited to, aircraft primary propulsion engines and auxiliary propulsion units, towing and service vehicles, mobile lounges, airport passenger and employee vehicles, power plants, incinerators, and evaporative emissions from storage farms. A functional representation which correctly describes the time-varying behavior of each source should be constructed. With the aid of the dispersion model, the contribution of each source to the pollutant concentration at points in the neighborhood of the airport can be determined. In this way, one can identify those sources where most of the efforts and funds should be expended to reduce emissions.

(11) The importance of pollutants emitted upstream of the airport and subsequently transported across the airport must be evaluated.

(12) Possible modifications of airport operations should be investigated to determine their feasibility for reducing pollution concentration levels. These modifications should consider ground vehicular operations as well as aircraft. Such obvious alternatives as using electrically powered vehicles to move aircraft on the ground or taxiing with one engine at intermediate power level, instead of with all engines operating at low power, can be studied as well as a multitude of other possibilities.

Langley Research Center,
National Aeronautics and Space Administration,
Hampton, Va., January 23, 1973.

APPENDIX

PHYSICAL MODELING

The wind tunnel and water channel are physical modeling techniques whose greatest asset is the ability to investigate dispersion for configurations too complicated to be mathematically modeled. Examples of such configurations are mountainous terrain, an urban building complex, and the downwash around individual stacks or buildings. Physical models can also offer guidance in placing instrumentation for field studies. Reference 111 presents several papers dealing with the current aspects of physical modeling.

Wind Tunnels

Wind tunnels, a familiar similarity modeling tool for aeronautical research, are also used by the meteorological fluid dynamicist. Some of the features of a meteorological wind tunnel that differ from the features of conventional aeronautical wind tunnels are long test sections, flexible ceilings, and thermal control of the fluid and tunnel floor. The long test sections are required to build up the proper turbulence structure and to obtain a homogeneous shear layer to simulate the atmospheric boundary layer. The flexible ceiling is needed to maintain a zero pressure gradient in the flow. Thermal control of the fluid and the tunnel floor enables the simulation of thermal stratification that occurs in the atmosphere.

The use of aeronautical wind tunnels for meteorological investigations has received impetus from studies at Cornell Aeronautical Laboratory. (See ref. 112.) The requirement for extremely long test sections has been somewhat relaxed by inducing turbulence with fins, grids, fences, and other obstacles in the path of the flow. However, achieving the desired turbulence concurrently with the desired mean velocity profile remains difficult in some flows. Meteorological wind tunnels are especially suited for simulating weak winds and stable atmospheric stratification which accompany the most serious air pollution episodes.

Reference 113 provides a short introduction to wind-tunnel modeling of atmospheric flows. Photographs are presented which qualitatively demonstrate some of the applications for which the wind tunnels have been used. A more in-depth discussion which includes quantitative results and pertinent similarity parameters is given in references 112, 114, and 115.

Meteorological wind tunnels have been used for studying structural wind loading, planning topographical modification, determining placement of field instrumentation, simulating dispersion about isolated structures, and studying intermediate scale (10^2 to 10^5 m) streamline patterns in stratified flows. However, in only one instance has an entire urban area been modeled (ref. 113, p. 40). In this case, a model of Fort Wayne, Indiana, was placed in the Colorado State University meteorological tunnel, which is one of the larger such tunnels in operation. As larger meteorological wind tunnels are constructed, more physical modeling of entire urban areas will be attempted.

Water Channels

Because of the increased fluid density, water channels yield an order of magnitude higher Reynolds number than wind tunnels for a flow of the same speed. Since the atmosphere is characterized by large Reynolds numbers, the water channel has an advantage over the wind tunnel in this respect. Also, flow visualization is easier in water than in air. However, simulating atmospheric buoyancy effects in liquid flows is more difficult than in air.

Vadot (ref. 116) has studied atmospheric diffusion with liquid flows. Clark (refs. 117 and 118) used a water channel to study the clear-air turbulence associated with mountain lee waves. Facy (ref. 119) has reported on some promising diffusion simulation experiments in water. Urban modeling has not been done in water channels to date. Perhaps the most obvious reason is the size of the facility required to accommodate an urban area model.

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