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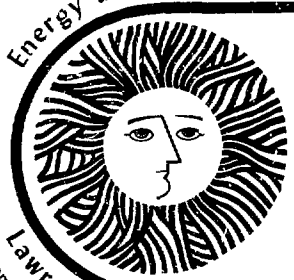

A Review of Air Quality Modeling Techniques

Leonard C. Rosen

January, 1977

Lawrence Berkeley Laboratory University of California/Berkeley

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Energy and Environment Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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Vol. 1: "Health and Safety Impacts of Nuclear, Geothermal, and Fossil-Fuel Electric Generation in California: Overview Report," by the entire staff, Lawrence Berkeley Laboratory Report LBL-5924. Includes "Executive Summary" for the project.

Vol. 2: "Radiological Health and Related Standards for Nuclear Power Plants," by A.V. Nero and Y.C. Wong, Lawrence Berkeley Laboratory Report LBL-5285.

Vol. 3: "A Review of Light-Water Reactor Safety Studies," by A.V. Nero and M.R.K. Farnaam, Lawrence Berkeley Laboratory Report LBL-5286.

Vol. 4: "Radiological Emergency Response Planning for Nuclear Power Plants in California," by W.W.S. Yen, Lawrence Berkeley Laboratory Report LBL-5920.

Vol. 5: "Control of Population Densities Surrounding Nuclear Power Plants," by A.V. Nero, C.H. Schroeder, and W.W.S. Yen, Lawrence Berkeley Laboratory Report LBL-5921.

Vol. 6: "Health Effects and Related Standards for Fossil-Fuel and Geothermal Power Plants," by G.D. Case, T.A. Bertolli, J.C. Bodington, T.A. Choy, and A.V. Nero, Lawrence Berkeley Report LBL-5287.

Vol. 7: "Power Plant Reliability-Availability and State Regulation," by A.V. Nero and I.N.M.N. Bouromand, Lawrence Berkeley Laboratory Report LBL-5922.

Vol. 8: "A Review of Air Quality Modeling Techniques," by L.C. Rosen, Lawrence Berkeley Laboratory Report LBL-5998.

Vol. 9: "Methodologies for Review of the Health and Safety Aspects of Proposed Nuclear, Geothermal, and Fossil-Fuel Sites and Facilities," by A.V. Nero, M.S. Quinby-Hunt, et al., Lawrence Berkeley Laboratory Report LBL-5923.

A REVIEW OF AIR QUALITY MODELING TECHNIQUES

ABSTRACT

Categories of transport and diffusion models which are applicable to the assessment of the environmental effects of nuclear, geothermal and fossil-fuel electric generation are reviewed. The general classification of models and model inputs are discussed. A detailed examination of the statistical, Gaussian plume, Gaussian puff, one-box and species-conservation-of-mass models is given. Representative models are discussed with attention given to the assumptions, input data requirement, advantages, disadvantages and applicability of each.

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A REVIEW OF AIR QUALITY MODELING TECHNIQUES

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January 1977

1. INTRODUCTION

The assessment of the health and safety impacts of emissions from any source requires the utilization of some air quality modeling technique to determine the effects of these emissions at a variety of receptor locations. To date, a large number of transport and diffusion models have been developed which purport to accomplish this task. In general, however, the processes involved in transporting pollutants from one location to another are extremely complex. These include the advection of constituents by wind, turbulent diffusion, possible chemical reactions, wet and dry deposition of pollutants, and the effects of topography and variations in vertical mixing. In order to determine the consequences of air pollution, it is necessary to establish a methodology which makes optimum use of air quality models under a variety of physical and meteorological conditions. The models developed heretofore utilize some mathematical technique to represent the actual physical processes of air pollution transport in a workable fashion. Some of the simplest of these represent only the most elementary approximations to the problem. However, these techniques may

be useful to evaluate air quality in specialized circumstances. On the opposite side of the spectrum are those models in which the transport processes are represented by sophisticated algorithms and mathematical methods which generally require a more extensive use of the computer. No one model is applicable, though, to all sources, regions, or spatial scales of assessment. The decision as to which model to use in a particular situation must be weighed through the consideration of the advantages and limitations of each coupled with the time, cost and computer resources of the user. In the following sections, these aspects of air quality modeling are examined in the following manner. In Section II, the general classifications of models are discussed. Section III summarizes the inputs to transport and diffusion models. Sections IV and V provide a detailed examination of the statistical, Gaussian, one-box and species - conservation-of-mass models. Within these sections, representative models are noted, with particular emphasis on their advantages, disadvantages and applicability. At the end of the final section, a table is given which summarizes the salient features of the individual models discussed within this report.

II. GENERAL CLASSIFICATION OF MODELS

A. SPATIAL AND TEMPORAL SCALES

There exists at present an extensive variety of transport and diffusion models potentially useful in the evaluation of air quality. Each of these, however, is not applicable to the same type of problem. In particular, the space and time scales of any one model are generally set to provide solutions for a specific class of air pollution assessments. Spatial scales may vary from less than one meter for models directed to the emissions from roadways to that of hundreds of kilometers for those models which consider the interactions of urban and regional areas. Similarly time scales vary from less than one hour to several days. It is fortuitious, at least for the sake of classification, that the spatial and time scales are coupled to the same order due to the requirements of time and distance resolution.

A useful classification of scales is given by:[1]

1. Microscale roadway impact model ($\sim$ .1 km; 10 min.-1 hr.).
2. Large point source (e.g., power plant stack) ($\sim$ 10 km; 1 hr.).
3. Urban regional model ($\sim$ 50 km; 1 hr-several hrs.).
4. Urban/regional model ($\sim$ 300 km; 1 hr-1 week).

In general, models are developed so that the temporal resolutions will be consistent with critical air quality standards established for various averaging periods of measurements.

A broader classification of scales in wide usage divides models into two-divisions: mesoscale models and microscale models. The former are

those in which the sources and temporal scales extend over counties, air sheds and urban areas; the latter include those models in which the scale of resolution is approximately 10 metres or less. In terms of the categories stated above, microscale models would include both point source and roadway impact models.

B. EMPIRICAL AND DETERMINISTIC MODELS

Air quality models may be further classified by the specific technique utilized within the models to predict the impact of air pollution at receptor sites. In the broadest such subdivision, one may speak of empirical or deterministic models. Within this section, a brief summary of these techniques is given to afford the reader a general overview of such models. The details and specific examples of these model-types are discussed further in the following pages in Sections IV and V.

Empirical models are those in which a historical data base is used to develop a functional dependence between source emissions and air quality. These models, termed statistical and rollback type models,[2] assume some proportional relationship between the rate of emissions and atmospheric pollution levels. In its simplest form, the proportionality is taken to be strictly linear. These linear rollback models maintain their validity, therefore, only for those circumstances in which the pollutants in question do not undergo chemical reactions in the atmosphere and for those cases in which no significant temporal or spatial distributions in emissions occur during the averaging time. Some statistical and rollback models have been developed which consider a non-linear pro-

portionality and further attempt to make adjustments for geographical and temporal variations in emissions.[3] The most important advantage of statistical rollback models is their mathematical simplicity. However, inherent in the simplicity is the neglect of the complex meteorological, physical and chemical factors which determine air quality. Further, these models require an extensive historical data base relating emissions to atmospheric pollution for each specific location or region to which the models will be applied.

The second class of methodology employed in predicting atmospheric pollution are those utilized in deterministic models. These are models in which a mathematical relationship is used to represent the actual processes involved in establishing air quality. In contrast to empirical models, in which past data is used to statistically relate emissions to resultant pollutants, deterministic models are predictive through the use of quantitative expressions which are in general solved to yield the pollutant concentrations at receptor sites. In theory, the full scope of hydrodynamic and chemical kinetic equations relevant to air quality modeling is generally known. In practice, however, the complete set of equations is intractable to solution within the finite time limits set by even the fastest present day computers. Therefore, deterministic models employ some approximations of the full set of equations to simulate air quality.

Most models utilize a combination of fundamental principles and statistically derived parameters. The complexity of air quality models available at this time varies to the degree in which attempts are made to solve the full set of fundamental equations and in which provisions are

made to include variability in meteorological, physical and chemical processes. Those models which allow for variability are termed dynamic models, those which do not are categorized as steady state models.

The most elementary semi-empirical transport and diffusion models are of the simple box type or follow a Gaussian formulation. The one box models are those in which the constituent pollutants are assumed to be uniformly mixed throughout a single volume or box of air.[4] The boundaries of these models are therefore determined horizontally by the geographical scale of the region considered and vertically by the surface terrain and the height of the inversion base. Since uniform mixing of pollutant sources normally occurs over dimensions of the order of 5 to 10 kilometres, simple box models are appropriate to use only in those circumstances in which spatial averages over large source areas are to be considered or in estimating air quality in regions far removed from large local sources.

Gaussian plume models are those models in which the concentrations are taken to be normally distributed (Gaussian) about the plume centerline. In their most elementary form, Gaussian plume models are steady state with assumptions of a uniform horizontal wind, a constant point source, neglect of diffusion in the direction of the wind and no provision made for chemical reactions or loss mechanisms. The dispersion characteristics of these models enters in the form of parameters which must be evaluated empirically. Modifications of the basic Gaussian plume model allow for simple decay of the pollutant and deposition loss at the terrain surface. The effect of a mixing layer (below inversion base height) on the Gaussian distribution has been considered in some models through the use of interpolation techniques and the assumption of reflec-

tion at the inversion base.[5] The Gaussian plume model has been extended for use with multiple point sources, line sources and area sources by essentially employing the basic Gaussian plume point source formula to sum the contributions from individual sources. Such multiple point source formulations are therefore valid only for those situations in which the sources are approximately constant in strength throughout the region considered. Further, the technique of superposition of individual sources is applicable only to non-reactive constituents. The major advantage of the Gaussian plume model is in the simplicity and ease of application. However, the model is deficient for circumstances in which sources and meteorological conditions vary, species are chemically reactive, topography is not relatively flat, and horizontal wind speeds are less than about two miles per hour.

Gaussian puff models have been developed to remedy some of the deficiencies present in the Gaussian plume models. In particular, these models allow for the time variation of the horizontal wind, the source emission rate, and the dispersion parameters. This is accomplished by tracking and integrating the instantaneous puffs from a point source whose strength may change at each instant of time. These models have been extended as in the case of plume models to include the effects of multiple point, line and area sources. A fundamental computational difference exists, however, between the Gaussian plume and puff formulations. In the plume models, the concentrations are determined at each point in a fixed coordinate network termed an Eulerian grid. In the puff models, each instantaneous emission is tracked by carrying the coordinate system along with each puff. This frame of reference is known as a Lagrangian coordin-

ate system. Inherent in all such Lagrangian approaches is the requirement that one follow the concentration along a preestablished wind trajectory. Therefore, to determine the concentration at a point one must determine the trajectories of all parcels which will pass over any given receptor site. The Gaussian puff model has the advantage over the plume model in that allowance is made for some time variation in the variables of the problem. The models require a computer but are still fairly simple to use when considering single point sources. However, the computational times become lengthy if the model is used for multiple sources or for a sheared single cloud for a variety of trajectories. In addition, the Gaussian puff model has the same disadvantages as the plume model in that the terrain must be fairly flat and the constituents non-reactive.

A simplified class of models has been developed by the Atmospheric Turbulence and Diffusion Laboratory (ATDL) of the National Oceanic and Atmospheric Administration (NOAA) which combines some aspects of the single box model with that of the Gaussian plume model.[6-8] By integrating a Gaussian line source over a given volume, ATDL has developed a non-reactive model in which the concentration of a pollutant is simply proportional to the local area source strength and inversely proportional to the wind speed. The proportionality constant in this expression is itself proportional to the average width of the region, inversely proportional to the average depth of a plume released at the surface within the region and is assumed constant for a given atmospheric stability. The chief advantage of this class of models is its simplicity and ease of application for use in averaging non-reactive concentrations over large areas for long averaging times. However, should the spatial and temporal scales of

averaging be too small, the model will neglect the effects of important sources and variations in source strengths. The ATDL model has been extended to include chemically reactive pollutants.[9] This has necessitated the utilization of five parameters within the model as compared to one for the non-reactive model. This thereby reduces the generality of the model and requires the reevaluation of the parameters for different meteorological conditions and emission mixes and strengths.

Species-conservation-of-mass models encompass those transport and diffusion models which yield the time-varying concentrations of air pollutants as solutions of the fundamental mass conservation equation. These dynamic models compute the time variation of consitiuents as a function of wind speed, turbulent diffusion, source emissions and in some cases deposition and chemical reactions. Allowance is made in these models for the temporal and spatial variation of sources and meteorological conditions. Whereas the previously discussed models are either analytic or require limited computer use, except for the multi-source puff models, species-conservation-of-mass models generally necessitate extensive computer resources and large quantities of spatially and temporally resolved meteorological and source emissions data. However, these models represent the most sophisticated class of models available at present to evaluate air quality.

Species-conservation-of-mass models may be classified by the mathematical technique utilized in their solution: finite-difference; particle-in-cell (PIC); and Lagrangian. Finite-difference techniques employ an Eulerian grid in which the region to be modeled is divided into cells, usually of a fixed, uniform volume. This region is generally divided into

a number of horizontal cells and one or more vertical elements extending from the terrain surface through the lower atmosphere, usually bounded by the inversion layer. The concentrations of the pollutants within each volume element are calculated by computing the net flux across each element due to advection, diffusion, sources and sinks and may include chemical reactions. The size of each cell is determined by the extent of the region to be modeled, the accuracy required by the numerical approach utilized, and the number of constituents and possible chemical reactions included. These considerations are bounded by the storage and time capabilities of the computer and the spatial resolutions of the meteorological and source emission inputs.

The finite-difference technique may be employed in the solution of Eulerian grid multicell models. For such models, the concentrations are taken as uniformly mixed within each volume element. This assumption leads to a numerical difficulty known as artificial diffusion. To overcome this problem of lessened accuracy, Eulerian grid multicell models require some specialized mathematical approach. Although the degree of numerical complexity is increased thereby, these models have the advantage of allowing the incorporation of a set of chemical reactions to represent the air pollution chemistry associated with the region.

PIC models are those in which marker particles are used to represent a given mass of pollutant within an Eulerian grid. The time variation of the pollutants is determined by computing the number of particles which are transported by wind and turbulent diffusion into each fixed volume element. The concentration of each pollutant is then found by summing the contribution of the particles within each cell. This method has the

advantage of eliminating or reducing significantly the problem of numerical diffusion. However, this technique requires the use of large numbers of marker particles to adequately represent the constituents to be modeled, thereby necessitating the use of computers with extensive memories. This difficulty is further extended if even a simple set of chemical reactions is included. Therefore PIC models are most appropriately used for a small number of non-reactive or simply decaying pollutants.

Dynamic Lagrangian or trajectory models are those models in which the time variation of pollutants is determined by computing the concentrations within a fixed volume box moving along a given wind trajectory. These models often utilize one or more vertical cells which extend from the terrain surface to the inversion layer. The time history of pollutants within a box will vary as a function of flow over sources, diffusion across cell boundaries and chemical transformations. Lagrangian models generally assume uniform mixing within each cell and usually do not provide for horizontal diffusion across the boundaries of each cell. The neglect of horizontal diffusion can be a significant limitation in regions in which there exist large gradients of emissions. The basic feature of trajectory models is the relationship of source and receptor. These models enable the identification of a pollutant measured as a receptor site with specific source emissions along the wind trajectory. However, there exists the concommitant disadvantage of requiring a large number of trajectories and therefore computer runs in regions of diverse wind fields and varying emissions. The Lagrangian model is therefore best suited for areas in which the meteorological conditions and distribution of sources are fairly uniform.

III. MODEL INPUTS

The models discussed within this report all require some inputs in order to predict the air quality of a particular region. In the following sections, inputs are enumerated separately under the categories of source emissions, meteorological data and chemistry and deposition. It should be noted that not all models utilize the same number of input variables or quantity of information. The requirements of individual models will be further discussed in the sections describing specific examples.

A. SOURCE EMISSIONS

The inventory of emission sources represents the most fundamental input to all models. Data representing the location, strength, relative contribution, and time variations of air pollution sources are necessary to provide a determination of ambient air quality. The more sophisticated transport and diffusion models utilize an extensive array of data whereas the elementary statistical models may require only the aggregated values, thereby reducing the quantity of information used. However, the need to identify the health and safety hazards associated with specific source events necessitates the use of a comprehensive emissions inventory with spatial and temporal resolutions appropriate to the regional dimensions and the air quality standards to be assessed. Typical spatial dimensions may be 1 to 2 km or less. Since air quality standards are given frequently

in terms of peak hourly averages, source emissions input data must also correspond to this time average to yield meaningful results.

Emissions may be classified as stationary, mobile or indirect. Indirect sources are a combination of stationary locations combined with mobile sources such as sports arenas and shopping centers. Stationary sources may be further subdivided into point and area sources. Area sources are generally those which are fairly uniformly distributed throughout a region such as the pollutant emissions from residential heating. However, it is sometimes the practice to include all stationary sources in the emissions inventory as area sources. Although this is the least costly way in which the inventory may be compiled, this technique suffers from the inaccuracies derived from neglecting the effects of individual significant point sources. Additional emissions information is required by those point source models which utilize a plume rise formulation which relates the rise of emissions near a stack to a number of thermodynamic and dynamic variables. Data must be provided which includes stack height and diameter, ambient air temperature, gas volume flow, and gas temperature.

B. METEOROLOGICAL DATA

All non-statistical models require input describing the wind fields which transport pollutants. The most elementary Gaussian models utilize only a single value of wind speed and direction, constant in time. Indeed these simple formations cannot use complex data on variable wind fields even if available. For these models, the choice of the uniform wind may be made by averaging over several wind monitoring stations or using the

observations from one location. More sophisticated models employ values of wind speed and direction for each computational cell. These are typically averaged over a one-hour period. In general, there will be few wind monitoring stations in a region available to provide data for the entire grid to be modeled. A technique is therefore required to yield the point-to-point values of the horizontal and vertical winds. Some models employ separate methods to evaluate the vertical and horizontal dependence of the winds.[10] Variations of horizontal winds in the vertical direction are obtained through functional relationships, typically a power law of the form $u \alpha z^n$; the horizontal dependence may be obtained separately by a mass-consistent wind field analysis. The most sophisticated approach to interpolating wind fields to date employs a three-dimensional mass-conserving method, a technique utilized by the MATHEW wind model.[11] This model applies a variational approach to the basic three-dimensional equation of continuity for incompressible flow yielding the Euler-Lagrange equations for the velocity potential. This gives a best least squares fit to the observed data while providing a non-divergent wind field. Topography and measurements of the inversion base height are introduced so that the wind field satisfies the continuity equation between these boundaries.

The utilization of hourly wind data for complex regional models necessitate that a computational interpolation technique be employed for each hourly input set. The number of such calculations can become quite large and costly in terms of computer time. Further, the assessment of air quality require a choice of some "typical" wind data sets for a region. A technique which reduces these problems is that of principal components analysis (PCA) which has been developed to determine seasonal and diurnal

patterns in the wind data.[12,13] This method computes the orthonormal eigenvectors of a data matrix consisting of a number of simultaneous wind observations at a variety of wind monitoring stations. The eigenvectors represent the patterns within a region. In those cases in which a pattern is repeated, only a few eigenvector are required to describe the wind field. Thus, PCA is a method which isolates the regional patterns and compactly represents it in terms of a truncated set of eigenvectors.

In addition to requiring topography and inversion base height information for the construction of wind fields, some models need this data explicitly to establish boundary conditions. The most elementary Gaussian models have no provision for this data, thereby reducing their applicability to virtually level terrain in circumstances in which the inversion layer is not present or has limited effect on the transport and diffusion of pollutants. The more sophisticated Gaussian models, which consider reflection and some deposition at the boundaries, require input data on the inversion base height. Data on topography are generally not employed so that these models are also valid only for use in regions of fairly level terrain. Some of the most sophisticated species - conservation-of-mass models utilize topography and inversion base height data. Since the mixing depth is in general not known for all times and points within a computational grid, an interpolation scheme is employed to give the required spatial and temporal variations of the inversion base height. Boundary conditions also enter into consideration of background concentrations. In species-conservation-of-mass models, in which turbulent diffusion depends upon the gradients of concentrations, it is generally assumed that the mass flux across boundaries is zero and that the initial concentrations are uniform in height above the terrain surface.

The turbulent eddy mixing associated with the small scale wind motion enters into dispersive models through the specification of the diffusion parameters. There are two approaches presently employed to characterize the diffusive properties of pollutants through the atmosphere: designation of the standard deviations used in Gaussian formulations and K-theory, employed in species-conservation-of-mass models. The technique used to prescribe the standard deviation makes use of the stability class associated with a particular set of meteorological and physical variables.[14-16] Stability class is designated by six categories from A for the most unstable through F for the most stable in which the least mixing occurs. Using observations, these have been related to such variables as wind speed, solar insolation or cloud cover, vertical temperature gradients, wind angular fluctuations, and the Richardson number. A set of empirical curves has been developed which gives the values of the standard deviation of a plume for each stability class as a function of downwind distance from the source. Thus, for a given stability class, one may read these directly from input entered in the form of charts or tables.

K-theory is utilized in species-conservation-of-mass models by designating the values of the horizontal and vertical eddy diffusivities, K_H and K_v, and applying Fickian diffusion. This approach assumes that the turbulent flux of a constituent is proportional to the product of the eddy diffusivity and the concentration gradient of the species in a given direction. This technique allows a greater versatility in specifying the eddy diffusivities in a model, although usually requiring greater computer time. A number of ways of specifying the eddy diffusivities have been employed in various models. These vary in complexity from assuming K_H and

K_v are given constants to establishing a functional relationship for the K's which may be dependent on surface roughness, wind speed, heat flux, height, eddy dissipation rate and Richardson number.

C. CHEMISTRY AND DEPOSITION

The rates of most chemical transformations which occur in the atmosphere are proportional to the product of the concentrations of two or more interacting constituents. The non-linearity of these processes cannot be included in Gaussian models which at most describe the loss rate of a pollutant through a simple first order decay constant. Models which calculate chemical reactions are of the species-conservation-of-mass type. These compute the time rate of change of each atmospheric pollutant through inclusion of the chemical kinetics in the basic mass continuity equation. This results in solving coupled partial differential equations for the set of constituents in a chemical reaction network. The complexity and scope of this problem therefore involves a substantial capability in computers and computer storage. One approach to reducing this problem is to minimize the number of chemical reactions by including only the most important processes and by using a lumped-parameter approach. This is a technique by which a group of reactions is described by a single rate constant linking the product species to those involved in the initiating reaction. The number of reactions which may be considered in present air pollution models varies from as few as three to as many as 50 for the LIRAQ-2 model developed at Lawrence Livermore Laboratory.[17] Those models which utilize chemistry require as input a set of reaction rates which may

vary as a function of temperature or time of day in the case of photochemical reactions.

The loss of pollutants through wet and dry deposition is included in some models. The data supplied to these models are the dry deposition velocities and rainout parameters. Dry deposition velocities are generally a function of the roughness and nature of the terrain for a given species. Rainout and washout depend on the efficiency of raindrops and clouds in consuming constituents, the amount of clouds and the frequency of rains.

IV. STATISTICAL AND ROLLBACK MODELS

The most basic form of rollback model relates the ambient concentration of a specific pollutant at a given point to the background concentration and the total emissions rate in the area through the linear relationship[18,19]

$$c = b + ke \quad . \tag{1}$$

In this expression, c is the concentration of one pollutant, b is the background concentration of the pollutant for air uncontaminated by nearby emitters, e is the total emission rate of all emitters of the constituent within the region modeled, and k is a proportionality constant dependent on all meteorological and physical factors which relate the emissions to the concentration of pollutant at the receptor site. This formulation leads to the following expression in linear rollback which is utilized to maintain air quality standards

$$R = \frac{(GF)\ (PAQ) - (STD)}{(GF)\ (PAQ) - b} \tag{2}$$

where R is the fractional reduction in emissions required, GF is the growth factor, PAQ is the present air quality, STD is the air quality standard and b is again the background concentration. The assumption of linearity in this form of rollback has validity only when applied to stable pollutants such as carbon monoxide. Modifications of this approach to account for reactive contaminants have been introduced by relating the pollutant concentrations to emissions through a set of curves or graphs. This method

of modified or non-linear rollback has been applied to the Los Angeles Basin by a number of groups to account for the pollutant-emission relationships of oxidants, nitrogen oxides and hydrocarbons.[20,21] The modified rollback technique, given in the EPA's Appendix J, makes use of emissions and contaminants data for selected cities to provide a relationship between peak, hourly averaged oxidant concentrations and hydrocarbon emissions. It should be noted that this method is limited in that it disregards the effects of natural pollutants and does not include provision for other important constituents which are a part of the photochemical process such as nitrogen oxides. Data derived from smog chamber analyses has been applied to non-linear rollback studies for the Los Angeles Basin[22] Although this method considers the joint interactions of nitrogen oxides as well as hydrocarbons in the photochemical process, it has not been shown that reaction chamber statistical studies may be directly applicable to urban areas. Further modifications of the non-linear rollback model include an analysis of the meteorological variables as well as concentrations and emissions.[23] These approaches suffer from the general limitation of statistical models in that they may be applied only to the regions in which the statistical analysis was performed.

Because it is in general not economically feasible to monitor pollutant concentrations continuously, some method is required to yield air quality data between sampling times. The technique most widely used for this purpose is the Larsen analysis[24] which assumes that the temporal distribution of pollutant concentrations is given by a lognormal distribution. That is, the logarithms of the concentrations for a given averaging time are distributed as Gaussian functions in time. Care must be exercised

when employing this technique in interpreting the air pollution concentrations in the tail of the distribution.

The most salient advantage of utilizing statistical models is in their simplicity and ease of application. Computer requirements are minimal or non-existent. However, the development of individual rollback models generally requires an extensive historical data base and statistical analysis by computer. The model produced for one area is not readily transferable to another region with different meteorological conditions, terrain and geographical and temporal distribution of sources. The elementary nature of rollback models neglects the complexity of physical and meteorological factors which relate emissions to air quality. The models do not account for the effects on air pollution produced by any one significant point source emitter. Therefore the use of rollback models is not particularly useful in the evaluation of the health and safety hazards associated with contaminants produced by individual fossil fuel, geothermal and nuclear sources.

V. DISPERSION MODELS

A. EQUATION OF MASS CONTINUITY

The basic equation governing the time-varying behavior of a given atmospheric constituent is given by the mass continuity equation

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} + w\frac{\partial C_i}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C_i}{\partial y}\right)$$

$$+ \frac{\partial}{\partial z}\left(K_z\frac{\partial C_i}{\partial z}\right) + R_i + S_i \quad . \tag{3}$$

In this equation C_i is the concentration of the i^{th} pollutant, u, v, and w are the x, y and z components of the mean wind field, K_x, K_y and K_z are the eddy diffusivities in each direction, R_i is the rate of change of C_i produced through chemical interactions and S_i represents the sources and sinks of the i^{th} constituent. Hence the time history of a given pollutant at any point in a region is governed by wind transport, turbulent diffusion, chemical reactions, and emission sources and sinks. An equation of this form can be written for each pollutant considered. The dispersion models enumerated in the following sections either utilize some approximation method or solve this set of equations directly by some mathematical technique. It is assumed in all cases considered here that the pollutants have no effect on the atmosphere. This in effect decouples the above equation from the full set of relationships which determine the atmospheric variables. Therefore a specification of the mean winds and the eddy diffusivities should yield a solution to these problems.

B. GAUSSIAN MODELS

1. Gaussian Plume Model

The Gaussian plume model is a steady state analytic solution to a simplified form of the mass continuity equation which takes the form

$$u \frac{\partial c}{\partial x} = K_y \frac{\partial^2 c}{\partial y^2} + K_z \frac{\partial^2 c}{\partial z^2} \quad . \tag{4}$$

This equation assumes only a mean wind in the x-direction and neglects chemical reactions, turbulent diffusion in the direction of the wind, and gradients in the eddy diffusivities. A single source of constant strength, Q, is assumed which may be related to the total flux of pollutant across a plane perpendicular to the direction of the wind. A formal solution to the above equation is given by

$$C = \frac{Q}{2\pi u \sigma_y(x)\ \sigma_z(x)} \exp - \left[\frac{y^2}{2\sigma_y^2(x)} + \frac{z^2}{2\sigma_z^2(x)} \right] \tag{5}$$

where the standard deviations of the resultant Gaussian solution may be related to the eddy diffusivities by $\sigma_y^2(x) = 2K_y \frac{x}{u}$ and $\sigma_z^2(x) = 2K_z \frac{x}{u}$. This equation assumes a single ground level source at the origin and a receptor at height z and horizontal distance (x,y). It may be extended to include a source at some height H above the terrain, reflection or absorption of the pollutant at the ground and a simple exponentially decaying loss mechanism. An analytic expression for the pollutant concentration due to a single source of constant strength which includes the above factors may be written

$$C = \frac{Q}{2\pi u \sigma_y(x)\,\sigma_z(x)} \exp\left(-\frac{\lambda x}{u}\right) \exp\left(-\frac{y^2}{2\sigma_y(x)^2}\right) \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z(x)^2}\right) + P \exp\left(-\frac{(z+H)^2}{2\sigma_z(x)^2}\right)\right] \quad (6)$$

where λ is the decay coefficient and P is the percentage of reflection at the surface. The above formulas lead to Gaussian distributions which expand indefinitely in the vertical direction with distance from the source. Pasquill[5] has considered the effects of an inversion on the plume and has developed a technique of limiting plume growth by estimating the degree of multiple reflections between the terrain surface and inversion height. Plume rise can be incorporated by utilizing some analytical expression such as those given by Briggs, Moore and TVA.[25-27]

The above analytic expressions may be extended for use with multiple point sources, line sources and area sources. Analytic expressions for line sources may be derived by integrating the point source equation over a continuous system of point sources of equal strength located in a direction perpendicular to the wind. In general, a numerical calculation by computer of pollutant concentrations due to unequal multiple point, line and area sources is required. However, the computational time and costs are minimal.

A large number of Gaussian plume models have been developed to date. Those which are available for use include the Continuous-Point-Source model (CPS) at Lawrence Livermore Laboratory,[28] the APRAC-1A, a multiple line source model intended for highway network analysis developed at SRI,[29] the BAAPCD models for use with major point sources and inter-county transport,[30] and several computer models available from EPA on the User's

Network for Applied Modeling of Air Pollution (UNAMAP). The UNAMAP models include CDM, a multiple point source and area source formulation, PTDIS, PTMAX, PTMPT, and HIWAY, which are single and multiple point source and single line source models.[31,32]

The advantages of Gaussian plume models include ease of application and simplicity. Computer requirements and costs are minimal. However, this class of models is applicable only to non-reactive or simply decaying pollutants. The models which assume a uniform wind which is constant in time are severely limited to applications in which time-averages are about one hour and spatial dimensions are less than 10 km. Gaussian plume models are not valid for wind speeds less than about 3 km per hour, conditions which may give rise to maximum concentrations due to given levels of emission. Further, these models are often applicable only to regions of fairly level topography.

2. Gaussian Puff Models

The Gaussian plume models described in the previous section assume that the meteorological conditions and source strengths remain uniform for a time sufficient to yield steady state concentrations of a pollutant. For situations in which the release of a constituent occurs for a short time or in which meteorological conditions may change significantly during the averaging time, a time-dependent formulation for the concentrations is required. The Gaussian puff model has this capability. The solution to the mass continuity equation for the conditions: an instantaneous release of pollutant of strength Q at time t; a wind only in the x-direction; and no chemical reactions or sinks is given by

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

$$\left. \frac{y^2}{2\sigma_y(t)^2} + \frac{z^2}{2\sigma_x(t)^2} \right] \quad . \tag{7}$$

It may be noted that since the expression is no longer proportional to 1/u, as is the case for Gaussian plumes, the solution is valid even for light winds. The formula may be extended, as was done for plume models, to include provisions for simple exponential decay, elevated sources and reflection and deposition at the terrain surface. Gaussian plume models utilize Eq. (7) or one modified by these factors to follow the time history of the puff as it is advected downwind. The contributions to the concentration at each instance of time are integrated in a frame of reference moving with the puff. The meteorological and source strength data may therefore be updated continuously.

The use of a Lagrangian coordinate system in these formulations necessitates the use of a number of trajectories that are capable of transporting pollutants between any given set of sources and receptors. This technique allows for the identification of pollutant concentrations at a receptor site due to any specific source. However, the improper choice of a trajectory may neglect important contributions to the concentrations in that they will not be included in the wind path utilized. Gaussian puff models, therefore, have more severe computer requirements than plume models in order to both store a number of trajectories and to follow the puff history. This requirement is further enhanced when multiple point sources or line sources are used to solve for the concentrations at the receptor site.

A representative example of the Gaussian puff model is the Multiple Source Urban Atmospheric Dispersion Model which has been validated in its study of sulfur dioxide concentrations due to stationary sources in the Chicago, Illinois metropolitan area.[33] This model was found to have greater versatility and generally more accuracy than the Gaussian plume model. However, its application required significantly more computer time. The Gaussian puff model represents a sort of halfway house between the plume models and the more sophisticated species-conservation-of-mass models. The benefits accrued from computing a more accurate time history of pollutant concentrations are mitigated considerably by the disadvantages of the models. These include extensive use of the computer, the neglect of chemical reactions and the inability to account for rough terrain. Computer requirements for Gaussian puff models, particularly for multiple sources, may be as severe as those for more sophisticated models.

C. ONE BOX MODELS

The fundamental assumption of one box models is that the pollutant concentrations are taken as uniform throughout the prescribed area. The region to be modeled is a single volume element or box of length L, width W and height H corresponding to the spatial dimensions and a constant inversion base height. Application of mass continuity to a source of strength Q within this box yields the following simplified expression

$$C = \frac{Q}{uHL} \tag{8}$$

where u is the component of the wind velocity that moves in a direction perpendicular to the side of length L.

The models developed by Gifford and Hanna at ATDL are essentially simplified one box models used to evaluate the effects of area sources. The concentration for a non-reactive pollutant is given by the formula

$$C = A \frac{Q}{u} \tag{9}$$

where Q is an area source strength and A is a constant dependent on the meteorological conditions prevailing in a particular region. The value of A is related to stability and can be expressed as a function of σ_z and K_z. Values of A vary from 60 to 600 with an average of 225 which corresponds to the D stability class of Pasquill. The model has been adapted to reactive species. However, the concentrations are then functions of five parameters which must be reevaluated for different regions and meteorological conditions.

The underlying assumptions of one box models argue strongly against their use to evaluate the impact of individual point source emitters. These models assume a fairly uniform distribution of sources throughout a region as well as an average uniform wind. Further, the models are not generally applicable to spatial dimensions less 5 to 10 km, the distances over which uniform mixing typically occurs.

D. SPECIES-CONSERVATION-OF-MASS MODELS

The models discussed in this section all compute the time-dependent concentrations of pollutants by directly solving the fundamental mass

continuity equation enumerated in Section V-A. These species-conservation-of-mass models are classified by the specific mathematical techniques employed in their solution: finite-differencing, Lagrangian, and particle-in-cell.

1. Finite-Difference Models

Finite-difference models employ an Eulerian grid such that the region to be modeled is subdivided into constant volume cells within a fixed spatial network. Algorithms are developed which give the time-dependent history of the pollutants by considering the net flux across the cell boundaries due to advection, turbulent diffusion, and sources and sinks. These formulations may include provisions for a set of chemical reactions.

The two most important finite-difference models developed to assess mesoscale air quality are the LIRAQ models at Lawrence Livermore Laboratory, the only model of its type approved for use in regional air quality programs by the California Air Resources Board,[34] and the SAI model developed at Systems Application, Inc.[35] The LIRAQ models use as input data the topography, meteorology and inventory of pollutant sources for the region to be modeled. A single vertical layer extending from the terrain surface to the inversion base height is utilized. Related processing models employ the meteorological and topographic data to internally compute self-consistent wind fields and the eddy diffusivities appropriate to the grid size. The LIRAQ models thereby calculate the temporal variations of the air pollution concentrations at the terrain surface and the mean concentrations for the vertical layer at each point of the horizontal grid. There exist at present two versions of the LIRAQ models. LIRAQ-1 employs an explicit

computational technique which is most appropriate for use with non-reactive constituents or for a set of simple chemical reactions. The LIRAQ-2 model, which has been successfully validated in the San Francisco bay region, utilizes a sophisticated set of computational algorithms capable of handling a large, general set of chemical reactions. At present, the model includes a complex set of chemistry which computes 50 reactions for 15 active constituents.

The SAI model utilizes three-dimensional finite-differencing which incorporates a technique of time splitting. The model requires as input the source inventory of pollutants, topography and meteorological data. Sufficient data must be supplied to adequately represent the three-dimensional wind field. A more limited set of chemical reactions is considered in this model as compared with the LIRAQ-2. The reaction network includes 16 reactions for 13 constituents using a lumped parameter approach. This model has been validated for use in the Los Angeles basin, but the lumped parameter approach may have to be recalibrated for other regions.

The use of finite differencing gives rise to a numerical inaccuracy known as artificial diffusion. A mathematical technique must be employed to overcome this problem. Some models utilize higher order differencing to minimize this effect. Two additional methods are available: flux-conserved transport[36] and material conserving computational procedures[37] This latter technique has been developed and employed by Egan and Mahoney in their EGAMA model[38] This model utilizes a two-dimensional Eulerian grid to compute the time history of non-reactive pollutants. The model has been verified only in comparison to Gaussian models. The method does not at present apply to reactive species.

The major advantage of the finite-difference class of models is their great flexibility in handling complex topography, variable meteorological conditions, a complex distribution of sources and chemical reactions. The limitations of these models are the extensive data bases necessary and the cost of using large, fast computers. For example, the LIRAQ-2 model takes approximately 45 min. to 1 hour of CDC-7600 computer time to compute the concentrations of 15 reactive constituents for a 24 hour simulation. However, these models represent the models sophisticated techniques developed to date to accurately calculate the temporal and spatial distribution of reactive pollutants.

2. Lagrangian Models

In Lagrangian models, the time history of pollutants is found by calculating the concentrations of the constituents as they are carried along the wind trajectory in a fixed volume of air. Hence, Lagrangian models employ a coordinate system moving with the wind as compared to a fixed set of coordinates in an Eulerian grid. Representative of this type of model is DIFKIN developed by the General Research Corporation, presently available for use on the Lawrence Berkeley Laboratory CDC-7600 computer,[39] and the REM model developed at Pacific Environmental Services.[40] The DIFKIN model neglects horizontal diffusion, but incorporates vertical diffusion. The model uses a highly simplified set of 16 chemical reactions. Input data required include a detailed source inventory, solar intensity, inversion base height and wind speeds and direction throughout the region considered. The REM model needs the same input as DIFKIN, but uses a more comprehensive set of 33 chemical reactions. However, REM employs the simplification of

utilizing only one vertical layer from the ground level to the inversion base in which mixing is assumed to be uniform. At present DIFKIN has been validated in the San Francisco bay region by SRI with some partial degree of success.[41]

The Lagrangian technique of solving the mass continuity equation has the major advantage of enabling the investigation of reactive pollutant transport for selected trajectories. The method has the basic advantages and limitations inherent in all trajectory models as discussed in earlier sections. That is, pollutant concentrations at a receptor site may be associated with specific source emissions. This necessitates that all important sources associated with potential trajectories be included in the assessment study. Lagrangian models may be employed for limited applications, thereby minimizing the use of computer time. However, the application of these models to large scale problems, utilizing a number of trajectories to assess the input of reactive pollutants, requires the use of data, computer time and memory that can become equivalent to that for the regional finite-difference models.

3. Particle-In-Cell (PIC) Models

The particle-in-cell approach employs marker particles which represent a fixed mass of pollutant within an Eulerian grid. The temporal history of the constituents may be found by computing the number of marker particles transported from volume element to volume element by the wind field and turbulent diffusion. The concentrations within each cell can be found by summing the individual particles. Models representative of the PIC technique are the ADPIC model developed at Lawrence Livermore

Laboratory[42,43] and NEXUS developed at Systems, Science and Software.[44] Both of these models are of the hybrid Lagrangian/Eulerian PIC type in which the coordinate system moves with the particles with a ficticious velocity dependent on the wind advection field and the gradients of the diffusivities. ADPIC requires the following input data: time-dependent and space-dependent source emission inventory; wind fields; topography; wet and dry deposition parameters; and inversion base height. Mass-consistent wind fields are supplied by the MATHEW Model, described in Section III-B. ADOUC may be applied to non-reactive or radioactive particles. This model has been successfully verified in several regional field tracer studies which include the methyl-iodine study at Idaho National Engineering Laboratory and the Ar plume study at Savannah River Plant.[45] NEXUS requires a similar source inventory, wind fields, inversion base height and solar intensity as input data. The model has been coupled with a simplified photochemical reaction network using lumped parameters. NEXUS has been verified against inert and photochemical pollutants in the Los Angeles basin, roadway networks in California and Oregon and point sources in Arizona and Oregon.[46] The model has been shown to be of limited value in predicting concentrations of reactive pollutants.

These PIC models have the advantage of greatly reducing numerical diffusion, particularly in applications utilizing non-reactive constituents. The major limitation of these models is the necessity of tracking large numbers of particles in order to adequately describe the concentrations of the pollutants. Extensive computer memory and time is required. Employing 10^4 particles and 10^4 grid elements ADPIC uses about 30 minutes of CDC-7600 computer time for an 8 hour simulation. Computer demands are increased

further for the inclusion of chemical reactions. The PIC technique is therefore best suited for applications in which the pollutants considered are non-reactive.

TABLE 1. Characteristics of Selected Air Quality Models

MODEL	SOURCE	TYPE	SPATIAL AND TEMPORAL SCALES/RESOLUTIONS	EMISSIONS INPUT	METEOROLOGICAL INPUT	ADVANTAGES	DISADVANTAGES
CDM	EPA (UNAMAP)	Gaussian plume, long term (monthly seasonal, annual) concentrations from point and area sources	urban/regional, 1 km^2 spatial resolution, annual or long term temporal resolution	major point sources and area sources as annual or long term average	joint frequency distribution of wind speed, direction and stability class as annual average, mixing height	ease and simplicity to apply, minimal computing time	assumes steady state conditions, can't be applied to light winds, rough terrain, does not include chemical reactions
PTDIS	EPA (UNAMAP)	Gaussian plume, single point source	microscale, point spatial values, hourly temporal resolution	emissions and source parameters for individual emitters	mean wind speed and direction, stability class	ease and simplicity to apply, minimal computing time	assumes steady state conditions, can't be applied to light winds, rough terrain, does not include chemical reactions
PTMAX	EPA (UNAMAP)	Gaussian plume, maximum 10 min. concentrations from single point source	microscale point spatial values, 10 min. temporal resolution	emissions and source parameters for individual emitters	mean wind speed and direction, stability class	ease and simplicity to apply, minimal computing time	assumes steady state conditions, can't be applied to light winds, rough terrain, does not include chemical reactions
PTMPT	EPA (UNAMAP)	Gaussian plume, up to 30 receptors from multiple point sources	microscale point spatial values, hourly temporal resolution	emissions and source parameters for individual emitters	mean wind speed and direction, stability class	ease and simplicity to apply, minimal computing time	assumes steady state conditions, can't be applied to light winds, rough terrain, does not include chemical reactions
BAYMOD	BAAPCD	Gaussian plume, multiple area source with complex terrain	urban/regional, 1 km^2 or greater spatial resolution, annual average temporal resolution with statistical frequency	local source inventory and total emissions by county	annual average wind speed for each grid, annual averaged wind direction frequency, wind strength for some sub-regions	handles area source inventory economically, ease and simplicity, little computer time	assumes steady state conditions, can't be applied to light winds, does not include chemical reactions
Gaussian Plume Models	BAAPCD	Has Models On-Line Equivalent to EPA's UNAMAP Series					
CPS	LLL	Gaussian plume, single point source	microscale, point spatial values, short term (e.g., hourly) temporal resolution	emissions and source parameters, radioactive decay parameter	wind speed as a function of height, building wake factor, stability class, dry and wet deposition parameters, topography as a function of distance from source	ease and simplicity to apply, minimal computing time, handles radioactive source and rough terrain	assumes steady state conditions, does not include chemical reactions, can't be applied to light winds

TABLE 1. (Cont'd)

MODEL	SOURCE	TYPE	SPATIAL AND TEMPORAL SCALES/RESOLUTIONS	EMISSIONS INPUT	METEOROLOGICAL INPUT	ADVANTAGES	DISADVANTAGES
Gifford & Hanna	ATDL	Gaussian plume/one-box area source	urban/regional, urban cell size, hourly temporal resolution	long term or annual average, or total for region	mean wind, stability class	simple and inexpensive	inability to handle variability of physical and meteorological processes, reactive model must be retuned for each region, unable to specify detail for large point sources
Rollback *Appendix J*	EPA	statistical	urban/regional, gives statistical frequency	total regional emissions	none	simple, easy to use, inexpensive	unable to handle variability of physical and meteorological processes, approximate technique not necessarily transferable to a variety of sites and meteorological conditions
Argonne Natl. Lab	AML	Gaussian puff	microscale point source and line source values, hourly temporal resolution	individual point or line source emissions inventory	wind speed and direction from nearest observing station, inversion base height	effective tool for evaluating selective trajectories	does not include chemistry, cannot be applied to rough terrain, large number of trajectories require extensive computer time
LIRAQ-1	LLL	2-D finite difference with vertical profile	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution for day and night runs	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, solar intensity	incorporates meteorological, physical and chemical processes into model	requires extensive data input, needs large, fast computers, limited chemistry
LIRAQ-2	LLL	2-D finite difference with vertical profile, includes chemical reaction *network*, 50 reactions for 15 active species	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution for day and night runs	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, solar intensity	incorporates meteorological, physical and chemical processes into model	requires extensive data input, large, fast computers
SAI	SAI	3-D finite difference	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution for 10 hour daytime simulations	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, solar intensity	incorporates meteorological, physical and chemical processes into model	requires extensive data input, large, fast computers
Shir & Shieh	IBM	3-D finite difference	urban/regional, 1 km^2 or greater spatial resolution, 2 hour temporal resolution	gridded inventory, temporal variations	wind speeds and directions for region from a weighted interpolation scheme, inversion base height, stability class	treats 3-D mass continuity equation	requires extensive data input, need large, fast computer, does not include photochemistry vertical wind direction assumed constant with height

TABLE 1. (Cont'd)

MODEL	SOURCE	TYPE	SPATIAL AND TEMPORAL SCALES/RESOLUTIONS	EMISSIONS INPUT	METEOROLOGICAL INPUT	ADVANTAGES	DISADVANTAGES
DIFKIN	GRC	2-D Lagrangian, includes 16 chemical reactions	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, stability class	includes photochemistry, effective tool for evaluating selected trajectories	horizontal diffusion neglected, lumped parameter chemistry, costly to run for large number of trajectories
REM	PEC	3-D Lagrangian, includes 33 chemical reactions	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, stability class	includes photochemistry, effective tool for evaluating selected trajectories	simplification of uniform mixing for one vertical layer, costly to run for large number of trajectories
ADPIC	LLL	3-D PIC, Lagrangian/Eulerian	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, stability class	elimination or reduction of numerical diffusion, comprehensive treatment of physical and meteorological processes, utilizes divergent-free, mass-cunsistent wind field model (MATHEW)	necessary to track large numbers of particles to adequately represent transport, requires extensive data and large computers, applicable only to non-reactive or radiative pollutants
NEXUS	SSS	3-D PIC, Lagrangian/Eulerian including simplified reaction network	urban/regional, 1 km^2 or greater spatial resolution, hourly temporal resolution	gridded inventory, temporal variations	wind speeds and directions for region, inversion base height, stability class	reduction of numerical diffusion, comprehensive treatment of physical and meteorological processes	necessary to track large numbers of particles to adequately represent transport, requires extensive data and large computers, chemistry inadequate

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