# URBAN AIR POLLUTION MODELLING

R.W. SIMPSON
Division of Australian Environmental Studies, Griffith University
Nathan Qld 4111, AISTRALIA

There is a range of urban air pollution models currently in use. Rollback and simple box models give crude estimates of the overall emission reductions required to avoid violations of long-term exposure health standards fors low-reacting pollutants. Gaussian plume models are used to predict both short-term and long-term exposures to pollutants arising from motor vehicles and large point sources such as power stations and mills. Multi-box models such as the ATDL model are used to predict long-term exposures from particulate pollution arising from a variety of point and area sources. Statistical models may be combined with these estimates to predict the number of violations of short-term exposure standards. Numerical grid square models are used to simulate photochemical smog episodes. In all instances, the models usually do not accurately predict the time of occurrence and location of the maximum pollution episodes. If the requirement of time and space pairing of predictions and observations is relaxed, then the models usually can predict the worst case pollution levels to within a factor of two, the best that can be expected from any model, given the inherent statistical uncertainty in air pollution measurements. However, many models require detailed data sets which are not always available, and severe local problems such as sea breeze effects and complex terrain complicate model performance and increase these problems.

## INTRODUCTION

The purpose of this paper is to critically examine air quality models for urban areas. There are many reviews which cover the broad spectrum of air quality models, including Hanna (1978, 1982), Drake *et al.* (1979), Turner(1979), Simpson and Hanna (1982), Hayes and Moore (1986), and Seinfeld (1988). This paper summarises these reviews. The classification of models chosen in this review is shown in Table 1.

Air quality models, sometimes termed air quality simulation models, are mathematical descriptions of the atmospheric transport, diffusion and chemical reactions of pollutants. They operate on sets of input data characterising the emissions, topography and meteorology of a region and produce outputs that describe the air quality of the region.

The air quality models can be classified as prognostic (that is, based on the fundamental physicochemical principles governing air pollution), and as diagnostic (that is, statistical descriptions of observed air quality data).

**TABLE 1: Different Model Types**

| Generic model type | Number of sources | Area types | Pollutants | Terrain complexity | Required resolution |
|---|---|---|---|---|---|
| *Grid* | | | | | |
| a. Region-oriented | Multiple source | Urban Rural | $O_3$, HC, CO, $NO_2$ (1-hour), $SO_2$ (3- and 24-hour), TSP | Simple Complex | Temporal Spatial |
| b. Specific-source oriented | Single source | Rural | $O_3$, HC, CO, $NO_2$ (1-hour), $SO_2$ (3- and 24-hour), TSP | Simple Complex | Temporal |
| *Trajectory* | | | | | |
| a. Region-oriented | Multiple source | Urban | $O_3$, HC, CO, $NO_2$ (1-hour), $SO_2$ (3- and 24-hour), TSP | Simple | Temporal Spatial (Limited) |
| b. Specific-source oriented | Single source | Urban Rural | $O_3$, HC, CO, $NO_2$ (1-hour), $SO_2$ (3- and 24-hour) | Simple Complex (Limited) | Temporal Spatial (Limited) |
| *Gaussian* | | | | | |
| a. Long-term-averaging | Multiple source Single source | Urban Rural | $SO_2$ (annual), TSP, $NO_2$ (annual)* | Simple | Temporal |
| b. Short-term-averaging | Multiple source Single source | Urban Rural | $SO_2$ (3- and 24-hour), CO, TSP, $NO_2$ (1-hour)* | Simple Complex (Limited) | Temporal Spatial |
| REFINED/SCREENING USAGE | | | | | |
| *Isopleth* | Multiple source | Urban | $O_3$, HC, $NO_2$ (1-hour) | Simple | Temporal (Limited) |
| SCREENING USAGE | | | | | |
| *Rollback* | Multiple source Single source | Urban | $O_3$, HC, $NO_2$ $SO_2$, CO, TSP | Simple | — |
| *Box* | Multiple source | Urban | $O_3$, HC, CO, $NO_2$ (1-hour), $SO_2$ (3- and 24-hour), TSP | Simple Complex (Limited) | Temporal |

* Only of $NO_2$ is taken to be total $NO_x$.

A general way to formally classify models is the following:

(i) Models that provide point solutions directly. They are explicitly solved for the air quality property under consideration, typically the (expected) pollutant concentration, and can be applied in a straightforward manner to any location in the region of interest without having to estimate concentrations at other locations. They include analytical formulae, the most common example being the Gaussian equation; and

(ii) Models that provide solutions only through (numerical) calculations over one-, two-, or three-dimensional domains. Photochemical air quality models fall in this category.

Air quality standards are written in terms of concentrations. In the USA, national ambient air quality standards (NAAQS) are set at a level determined to be appropriate to protect public health and well-being. Models are used for planning and assessing the attainment of these standards.

## MODELS FOR NON-REACTIVE POLLUTANTS

First, the models for non-reactive or slowly reacting pollutants are considered. The conservation of mass equation for an inert pollutant is given by:

$$\frac{\partial X}{\partial t} + \left( \bar{u} \frac{\partial X}{\partial x} + \bar{v} \frac{\partial X}{\partial y} + \bar{w} \frac{\partial X}{\partial z} \right) =$$

$$- \frac{\partial}{\partial x} < u'X' > - \frac{\partial}{\partial y} < v'X' > - \frac{\partial}{\partial z} < w'X' > + S \qquad \ldots (1)$$

where <...> refers to an ensemble average; X is the ensemble average of the concentration of the pollutant; $\bar{u}$, $\bar{v}$, and $\bar{w}$ are the mean wind speeds in the x-, y-and z-directions respectively; u′, v′ and w′ are the corresponding random components of wind speed; X′ is the random component of the concentration of the pollutant; and S refers to the source strength of the pollutants. The first three terms on the right-hand side of equation (1) refer to so-called turbulent diffusion. These terms are usually replaced by the gradient-transport representation, yielding an equation of the form:

$$\frac{\partial x}{\partial t} + \left( \bar{u} \frac{\partial X}{\partial x} + \bar{v} \frac{\partial X}{\partial y} + \bar{w} \frac{\partial X}{\partial z} \right) = \frac{\partial}{\partial x} K_x \frac{\partial X}{\partial x} + \frac{\partial}{\partial y} K_y \frac{\partial X}{\partial y} + \frac{\partial}{\partial z} K_z \frac{\partial X}{\partial z} + S \qquad \ldots (2)$$

where $K_x$, $K_y$ and $K_z$ are referred to as the eddy diffusivity coefficients for turbulent diffusion in the x-, y- and z-directions respectively.

## Gaussian methods

If the turbulence is homogeneous and stationary and only a point source is considered, then there is an analytic solution to equation (2), the Gaussian expression:

$$X(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp(-y^2/2\sigma_y^2) \exp\{-(H-z)^2/2\sigma_z^2\} + \exp\{-(H+z)^2/2\sigma_z^2\} \quad \ldots (3)$$

where Q is the source strength (mass emission rate), $\bar{u}$ the mean wind speed, $\sigma_y$ and $\sigma_z$ the standard deviations in concentration in the crosswind (y) and vertical (z) directions respectively, and H the effective height of emission. The wind is assumed to be in the x-direction. Veigele and Head (1978) have summarised assumptions needed to derive equation (3) from equation (2). The expression in equation (3) depicts a plume of effluent moving away from the source. Pasquill (1974) has reviewed relevant observational data regarding the validity of such a representation of pollution. The plume model is widely used for point sources and is also applied to line and area sources. Instead of viewing the pollutants as forming a plume, another approach adopted involves visualising "puffs" of pollutant which follow air trajectories and diffuse in a Gaussian manner. Conceptually, such a model is more widely applicable than the plume model, as light and variable meteorological conditions could be more easily treated, although the performance in practice is not always significantly better (e.g. see Lorimer, 1988).

## Box models

Box models are the simplest of the numerical models. The region to be modelled is treated as a single cell, or box, bounded by the ground on the bottom, the inversion base (or some other upper limit to mixing) on the top, and the east-west and north-south boundaries on the sides. The box may enclose an area of the order of several hundred square kilometres. Primarypollutants are emitted into the box by the various sources located within the modelled region, undergoing uniform and instantaneous mixing. The ventilation characteristics of the modelled region are represented, though only grossly, by specification of a characteristic wind speed and rate of rise of the upper boundary.

Fundamental to the box model concept is the assumption that pollutant concentrations in a volume of air, a "box", are spatially homogeneous and instantaneously mixed. Under this assumption, pollutant concentrations can be described by a simple balance among the rates at which they are transported in and out of the air volume, their rates of emission from sources within the volume, the rate at which the volume expands or contracts, the rates at which pollutants flow out the top of the volume, and the rates at which pollutants react chemically or decay.

Because of the formulation, box models can predict, at best, only the temporal variation of the average regional concentration for each pollutant species. Consequently, they are capable of addressing only multiple-source regional questions. Since box models lack spatial resolution, they cannot be used in situations where the meteorological or emissions patterns vary significantly across the modelling region. The combined effects of local emissions patterns and meteorological conditions generally give rise to significant spatial variations in pollutant concentrations.

**Grid, trajectory and particle-in-cell methods**

Grid models derive concentration levels by solving equation (2) numerically, using a horizontal, rectangular grid and a number of vertical levels. Conceptually, apart from the vertical levels, this approach appears to be similar to the multi-box-model one. However, there is an important difference in that grid models can consider horizontal diffusion explicitly.

Since a fixed grid is used, such an approach is referred to as Eulerian. Since the most serious errors in a numerical solution of equation (2) occur in the advection terms (the second term in square brackets on the left-hand side), then some people have suggested a Lagrangian approach where a cell is allowed to move through the atmosphere. The basic equation is now:

$$\frac{dx}{dt} = \frac{\partial}{\partial x} K_x \frac{\partial X}{\partial x} + \frac{\partial}{\partial y} K_y \frac{\partial X}{\partial y} + \frac{\partial}{\partial z} K_z \frac{\partial X}{\partial z} + S \qquad \ldots (4)$$

However, the cell would be distorted as it moves through the atmosphere due to local wind shear, and a distorted co-ordinate system is difficult to work with. So, instead of considering a continuous grid of cells, a single cell is considered and, using equation (4), the change in concentration in the cell may be calculated as it moves along the air trajectory. Models based on this formulation are referred to as "trajectory" models.

Since the required three-dimensional local wind data are usually non-existent, only horizontal wind fields can be used in the models. For a single cell, the turbulent diffusion term is ignored (quite often) or approximated from external data. The use of multiple cells requires approximations to avoid cell distortion, usually by ignoring wind shear. Seinfeld (1988) details these problems quite explicitly.

The errors inherent in smoothing the wind field and neglecting diffusion limit the applicability of such models. Also, the interpretation of the solution poses a problem, since observations against which model predictions are compared are only collected at a fixed point, while the model solutions refer to moving cells. Problems with the assumptions made in deriving grid and trajectory models are summarised in Table 2.

To avoid the difficulties of the Eulerian and Lagrangian formulations, a particle-in-cell (PIC) method has been suggested (e.g. Sklarew *et al.*, 1971). In this method, the mass of the pollutants is separated into individual elements and the centroids

of these discrete masses ("particles") are tracked. Eulerian cells are used to define mass averages (concentrations) based upon the number of particles in each cell at a given time. There are no distorted Lagrangian cells, yet the errors associated with first-order Eulerian methods are avoided.

Some models also try to predict the dynamic behaviour of the wind and temperature fields through the primitive equations (e.g. see Seinfeld, 1988). This introduces more numerical error into the calculations due to the increased number of calculations required and their increased uncertainties in input data.

**TABLE 2: Assumptions Made in Deriving Grid and Trajectory Models (after Liu and Seinfeld, 1975)**

| Model | Assumption | Magnitude of errors introduced (for typical urban conditions) | Possibility of rectification |
|---|---|---|---|
| Trajectory | Neglect of horizontal diffusion | Slight | Rectification not needed |
| | Neglect of vertical component of wind | Can be substantial | Excellent (but at the xpense of longer computing times and more data handling) |
| | Neglect of wind shear | Can be substantial | Difficult |
| Grid | Neglect of errors introduced through discretization | Substantial | Good (incorporation of more suitable techniques) |

### Rollback models

Rollback models assume that the pollutant concentrations are directly—though not necessarily linearly—proportional to emissions according to some simple relationship. Consequently, the emissions control requirements are presumed proportional to the amount by which the peak pollutant concentration exceeds the standards. The non-linearity of atmospheric processes limits the usefulness of such models to a screening role in which a first rough estimate is made of the emission controls required. Rollback methods lack spatial resolution and so are most useful for regional analysis of areas with many well-distributed sources of various types (e.g. see DeNevers and Morris, 1975).

## PHOTOCHEMICAL MODELS

Photochemical models have the additional simulation problem of chemical reactions.

### The EKMA model

The US Environmental Protection Agency recommends two approaches for formulating State Implementation Plans to achieve the NAAQS for ozone. The first

of these is the so-called city-specific Empirical Kinetic ModellingApproach (EKMA) (e.g. see Seinfeld, 1988). The other approach is the use of grid-based photochemical air quality models. The EKMA method was developed as a procedure to relate levels of peak ozone to levels of reactive non-methane organic compounds and oxides of nitrogen. The method utilises a set of isopleths that depict peak ozone concentrations as a function of the following parameters:

(i) Morning concentrations of ROG (reactive organic gases) and $NO_2$ (which may include precursors transported from upwind sources);

(ii) Emissions of ROG, $NO_2$ and other species occurring during the day;

(iii) Meteorological conditions; and

(iv) Reactivity of different ROG mixtures.

The ozone isopleths are developed through computer simulations using various assumed starting levels of ROG and $NO_2$. The isopleths are used to compute the percent reduction in emissions that is needed to lower the measured peak ozone to the NAAQS of 0.12 ppm.

The conceptual basis of the EKMA model is the trajectory model. This formulation assumes a parcel or column of air to be advected through an urban area based on the transport winds—usually the surface winds. The ROG and $NO_2$ within the column react chemically in accordance with the kinetic mechanism that is used in the model. A computer program has been developed to generate the ozone isopleths.

It is now widely recognised that the EKMA method is only appropriate for those regions that have a clearly definable urban core and a simple travel path to the point of downwind ozone maxima. Seinfeld (1988) states that the method should not be applied to a number of situations, especially the development control strategies for single or small groups of emission sources. Nevertheless, because the EKMA model or any trajectory model can contain the most detailed and up-to-date chemical mechanism, and at the same time retain its computational efficiency, it is well-suited to assess quickly the effectof ROG and $NO_2$ emission changes on ozone levels based on realistic chemistry.

### Grid-based photochemical models

Various types of gridded photochemical air quality models have been developed. They differ primarily in the number of atmospheric processes accounted for, the level of sophistication in their treatment of these processes, and the numerical procedures used to solve the governing system of equations. Examples of grid-based or airshed models that have been used to evaluate ozone control strategies are the Systems Applications Inc. Urban Airshed Model(UAM), the LIRAQ Model, and the California Institute of Technology Model (e.g. see Seinfeld, 1988).

Gas phase chemical reaction mechanisms for the atmospheric organic/$NO_2$ system have, as a result of many years of smog chamber and laboratory kinetic studies, reached a fairly advanced state of development. Available chemical mechanisms can be classified as *explicit* (or *detailed*) and as *reduced* (or *lumped*). Explicit mechanisms aim to account for the detailed actual chemistry of each species and intermediate. Typically, they involve several hundred reaction steps and are too lengthy to be incorporated in three-dimensional atmospheric models. For this reason, reduced or lumped mechanisms, generally involving fewer than 100 reactions, have been developed as systematic approximations of the detailed chemistry that is described by the explicit mechanisms.

As a result of EPA-funded programmes, two up-to-date chemical mechanisms for the formation of ozone in urban areas are presently available, one developed and tested by SAPRC/ERT (Statewide Air Pollution Research Center), and the second, the CBM-IV by Systems Applications Inc. (e.g. see Seinfeld, 1988). Both of these chemical mechanisms have been tested against the smog chamber data from the University of California, Riverside, and the University of North Carolina chamber facilities. The predictions of each of these chemical mechanisms agree with these environmental chamber data to within about 30 percent for ozone maxima and show varying levels of "reasonable agreement" for other measurements, and despite somewhat different approaches, both must be judged to be equivalently "good" at this stage. Results of comparison of the CBM-X and SAPRC/ERT mechanism are presented in Seinfeld (1988).

### The CSIRO IER model

Recently, the CSIRO Division of Coal Technology, Australia, has released a model which appears to be a significant improvement on the EKMA model. This model (e.g. see Johnson, 1984) is based on the integrated empirical rate (IER) model of ozone formation. This model incorporates a new measure of smog intensity, namely primary smog product concentration [PSP]. [PSP] is a measure of the amount of molecular oxygen dissociated by the smog reactions and its use greatly simplifies the description of smog formation. The model is derived from extensive measurements of smog formation in outdoor smog chambers from ambient concentrations of precursors.

## MODEL APPLICATIONS

### Gaussian plume models

In spite of the simplifying assumptions made in deriving the Gaussian plume formula and its weak verification by observational data, the formula given by equation (3) is widely employed; indeed, it is the basis for the United States Environmental Protection Agency (USEPA) models recommended for use by air quality managers (e.g. see Tikvart, 1978). One undoubted reason for this is the simplicity

**TABLE 3: Summary of Characteristics of EPA Gaussian Plume Models**

| Model | Reference | Predictions |
|---|---|---|
| Air Quality Display Model (AQDM) | TRW Systems Group (1969) | Monthly to yearly averages, shorter times using Larsen (1971) method |
| Climatological Dispersion Model (CDM/CDMQC) | Busse and Zimmerman (1973), Brubaker *et al.* (1977) | Monthly to yearly averages, shorter times using Larsen method (then referred to as (CDMQC) |
| Gaussian-Plume Multiple Source Air Quality Algorithm (RAM) | Turner and Novak (1978) | Hourly to daily averages |
| Single Source (CRSTER) Model | USEPA (1977) | Maximum concentrations from 1-hour to 24-hour averaging times, frequency distributions of concentrations |
| Texas Episodic Model (TEM) | Porter and Christiansen (1976) | 10-minute to 24-hour averages |
| PTMAX, PTDIS and PTMTP | Turner and Busse (1973) | PTMAX considers maximum concentrations, PTDIS all concentrations, PTMP multiple sources |
| PAL | Petersen (1978) | 1- to 24-hour concentrations from point, area and line sources |

of the formula; it requires little data to be collected for its use compared to other models which seek to improve on it.

The best known of the Gaussian plume models are listed in Table 3 and are part of the UNAMAP (User's Network for Applied Modelling of Air Pollution) system developed by the United States Environmental Protection Agency. Briggs (1975) has reviewed various plume-rise models and points out that plume rise is confidently predicted only for stable conditions.

Gifford (1976) has shown how the various schemes for $\sigma_y$ and $\sigma_z$ values are related and suggests that the interpolation formulas derived by Briggs (1974) incorporate the best features of these schemes (see Table 4).

Hanna *et al.* (1977) have reviewed the different stability classification schemes and corresponding $\sigma$ curves. Both reviews recommend that, wherever possible, the data for the standard deviations of wind direction, $\sigma_\theta$ and $\sigma_\phi$, be used to compute $\sigma_y$ and $\sigma_z$; the stability-classification-scheme approach should only be used when these data are not available. For instance, Carrasand Williams (1984) have identified new dispersion formulae appropriate for Australian conditions, especially tropical situations.

If a line source is viewed as an indefinite number of point sources, each yielding pollutant concentrations given by equation (3), then the pollutant concentration from a line source is obtained by integrating in the horizontal direction (y-direction). This is the basic assumption in most Gaussian plume approaches to line sources; for example, HIWAY (Zimmerman and Thompson, 1975) and the GM model (Chock, 1978) assumes line sources of infinite length. Sistla *et al.* (1979) conclude that models such as these yield reasonable estimates of CO and particulate pollutants, as have Darling *et al.* (1977) in their review of 13 models.

**TABLE 4: Briggs' Formulas (1974) [Formulas Recommended by Briggs for $\sigma_y(x)$ and $\sigma_z(x)$; $10^2 < x < 10^4$ m]**

| Pasquill type | $\sigma_y$, m | $\sigma_z$, m |
|---|---|---|
| Rural conditions | | |
| A | $0.22x\ (1 + 0.0001x)^{1/2}$ | $0.20x$ |
| B | $0.16x\ (1 + 0.0001x)^{1/2}$ | $0.12x$ |
| C | $0.11x\ (1 + 0.0001x)^{1/2}$ | $0.08x\ (1 + 0.0002x)^{1/2}$ |
| D | $0.08x\ (1 + 0.0001x)^{1/2}$ | $0.06x\ (1 + 0.0015x)$ |
| E | $0.06x\ (1 + 0.0001x)^{1/2}$ | $0.03x\ (1 + 0.0003x)^{-1}$ |
| F | $0.04x\ (1 + 0.0001x)^{1/2}$ | $0.016x\ (1 + 0.0003x)^{-1}$ |
| Urban conditions | | |
| A-B | $0.32x\ (1 + 0.0004x)^{-1/2}$ | $0.024x\ (1 + 0.001x)^{1/2}$ |
| C | $0.22x\ (1 + 0.0004x)^{-1/2}$ | $0.20x$ |
| D | $0.16x\ (1 + 0.0004x)^{-1/2}$ | $0.14x\ (1 + 0.0003x)^{-1/2}$ |
| E-F | $0.11x\ (1 + 0.0004x)^{-1/2}$ | $0.08x\ (1 + 0.0015x)^{-1/2}$ |

One of the major criticisms in using Gaussian plume models is the difficulty in incorporating deposition and settling effects. There are ways of incorporating deposition effects in the Gaussian plume model and Horst (1979) has reviewed a number of such models.

In Table 3, AQDM, CDM/CDMQ, RAM, TEM and PAL are urban models which consider pollution from a variety of sources. TEM uses the Gaussian plume approach for point sources and the Gifford-Hanna approach for area sources which is examined in the next section. RAM is used to calculate hourly to daily pollutant concentrations for point and area sources, and the computation of $\sigma_y$ is explicitly incorporated using equation (3); it is used for urban or rural areas (different stability schemes for each) and for flat, level terrain. PAL is similar to RAM, but includes line sources such as highways as well and is not designated for use for entire urban areas, but rather for portions thereof, such as shopping centres, airports and large

parking areas; level terrain is assumed. None of these models allows for complex terrain effects. VALLEY (Burt, 1977) is a Gaussian plume model for point and area sources in complex terrain, but only accounts for complex terrain effects quite crudely.

An AMS position paper on the accuracy of Gaussian models is summarised in Table 5, following Drake *et al.* (1979), and concludes that agreement between prediction and observation to no more than a factor of two should be expected.

**TABLE 5: Estimates of Accuracy for Diffusion Calculations (after Drake *et al.*, 1979)**

| Circumstances | Accuracy |
|---|---|
| POINT SOURCES | |
| *Ideal conditions*: near field (< 1 km), short averaging times (min to hr), flat terrain, steady meteorology, surface source | 10% to 20% |
| Same as above, except for elevated sources | 20% to 40% |
| *Real-world applications*: meteorological parameters reasonably well known and steady with no exceptional circumstances | Factor of two |
| *Exceptional circumstances*: wakes, buoyant plumes; varied surfaces, such as forests, cities, shorelines, rough terrain; extreme stable and unstable conditions; distances > 10 to 20 km | Poorer than factor of two; may be as poor as a factor of 10, or more |
| URBAN AREA SOURCES | |
| Ideal source and meteorological input data and conditions | 10% to 20% |
| Real-world applications with no exceptional circumstances | Factor of two |

The ATDL model has been developed by Gifford and Hanna (1971, 1973) and Hanna(1971), and is applied to urban area sources in which the emissions are assumed to be uniform over grid squares (of typical size 1-10 km). The pollutant is assumed to be well mixed to a height which is not the inversion layer, but given by vertical diffusion parameters varying with stability conditions.

Gifford and Hanna (1975) have suggested that the ATDL model works best for long-term averaged concentration values while, for short-term simulations, information about initial values of pollutant concentration should be used for calibration of the model—calibration is also recommended for long-term averages if the data are available. The application of the model to the prediction of annual TSP (total suspended solids) levels in Brisbane is shown in Figure 1. Where monitoring occurs in the grid squares, the accuracy appears to be within a factor of two (Simpson *et al.*, 1987).

An urban model which also combines all types of sources and is calibrated using Gaussian plume models in the Smeared Concentration Approximation (SCA) model

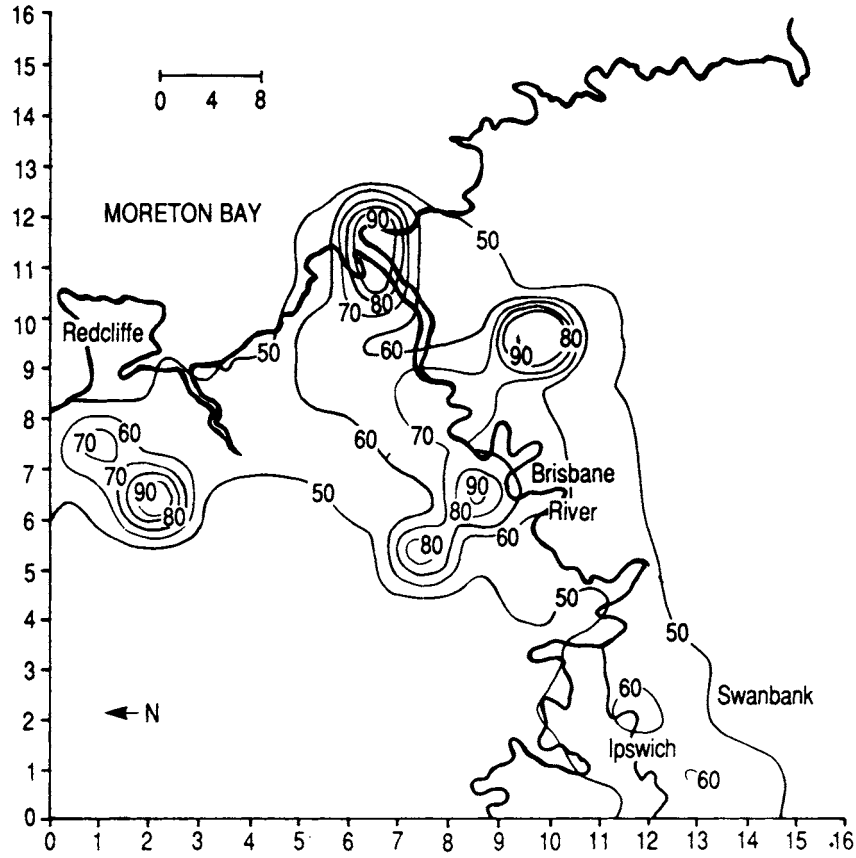


Fig. 1. Contour plot of mean total suspended solids (TSP) estimates (Simpson *et al.*, 1987).

(Dennis, 1978, 1980). This model has been used in both Europe andAustralia (e.g. see James *et al.*, 1985) as a convenient method for incorporating air quality objectives into integrated regional economic environmental planning strategies.

## Model performance measures

In 1980, under a co-operative agreement with the EPA, the AMS held a workshop on dispersion model performance at Woods Hole, Massachusetts to discuss current practices in the evaluation of dispersion model performance.

to recommend performance evaluation measures, and, if possible, to set performance standards for these models (Fox, 1981). Workshop discussion resulted in the recommendation of a set of performance measures to be used for evaluating the performance of different dispersion models.

The following measures of difference were suggested: the bias (average) of the difference (observed-predicted); the variance of the difference (noise); and the gross variability (gross error) of the difference.

These are actually related measures, because the sum of the square of the bias plus the variance equals the square of the gross variability. The following measures of correlation were suggested: time, space, and time and space combined. The recent reviews on model performance attempt to use these measures where possible.

The nature of current National Ambient Air Quality Standards and Prevention of Significant Deterioration increments requires that an extreme concentration value (highest, second highest) be estimated by models. Workshop participants agreed that the accuracy of highest or second highest estimates is expected to be poor and difficult to evaluate statistically. Statistical evaluations have greater meaning when applied to a relatively larger number of values than to one or two extremes. Generally, statistical evaluations applied to an upper percentile (2% or 5%) of the predicted values are more informative than those applied to only the highest or second highest prediction. Evaluations applied to estimates of mean performance will supply more information about overall model performance than will evaluations applied to extremes only. The workshop participants, therefore, recommended that the statistical form of standards and increments be changed to consider the upper 2% to 5% of concentrations rather than one or two extreme values.

Hayes and Moore (1986) present a comparative analysis of the results of 15 air quality model performance evaluation studies involving 35 rural, urban, complex-terrain and regional models. Of the 35 models studied, most (25) were Gaussian in formulation, including five long-term climatological models, three of which performed only long-term calculations (AQDM, CDM and TCM) and two of which make both long- and short-term estimates (MSDM and ERTAQ). The remaining ten models were numerical first-order-closure models (including three rural models, one complex-terrain model, and six regional models). The model applications focus on slowly or non-reactive pollutants, principally sulfur dioxide ($SO_2$) and TSP. Among study findings are the following:

(i) Flat-terrain rural models nearly always predict the second highest concentrations within a factor of two (often less), with no evidence of systematic overprediction or underprediction, but some models may underpredict the highest concentrations by more than a factor of two at distances far downwind (> 20 km);

(ii) None of the models accurately predicts spatial patterns of ≤ 24-hour-averaged concentrations, and while increasing the averaging time from 24 hr to annual improves performance for some models, it does not appear to do so for flat-terrain rural models; and

(iii) While some models appear to predict more frequent concentrations (e.g. 5th or 10th high, 95th percentile) better than they do the highest concentrations (e.g. 2nd high), no overall systematic tendency is evident.

## Combined deterministic statistical models

Since it is now acknowledged that urban models need to simulate concentrations frequency distributions in order to examine whether standards have been violated, a recent modelling approach has combined the deterministic ATDL model with assumptions about the form of the statistical distribution (e.g. see Simpson and Miles, 1989; Miles and Simpson, 1988).

To extend the ATDL model output to include annual maximum ground-level concentrations, and other statistics within the frequency distribution for the pollutant, a methodology has been developed over recent years which allows accurate estimates of pollutant concentrations corresponding to any statistic of the frequency distribution to be made, thereby relating the probability of exceeding set standards to control strategies. The generalised methodology developed has been outlined by the following steps:

(i) Assume/identify a statistical distribution for the air pollution concentrations;

(ii) Develop a deterministic model from available data, to predict a range of percentiles of air pollutant concentrations;

(iii) From the results in (ii), estimate the parameters of the statistical distribution assumed in (i); and

(iv) Using the parameters derived in (iii), construct a statistical distribution of air pollutant concentrations from which the estimates of high pollution levels can be obtained.

The results for the study in Brisbane are shown in Figure 2.

## Photochemical models

Seinfeld (1988) has summarised recent reviews of photochemical model performance as follows.

The overall accuracy of photochemical grid-model ozone predictions is currently about 35 percent when predictions and observations are paired in time and space. The errors in single-day simulations are somewhat less than for multiple-day runs. On the whole, grid-model ozone predictions tend to be biased low. Of the 63 single-day simulations surveyed, 70 percent exhibit a tendency toward underprediction of ozone. However, much of this trend may be due to "paired" comparisons; when the requirement for pairing in time and space is dropped, much of the underestimation disappears, which simply means that peak predicted values occur at somewhat different

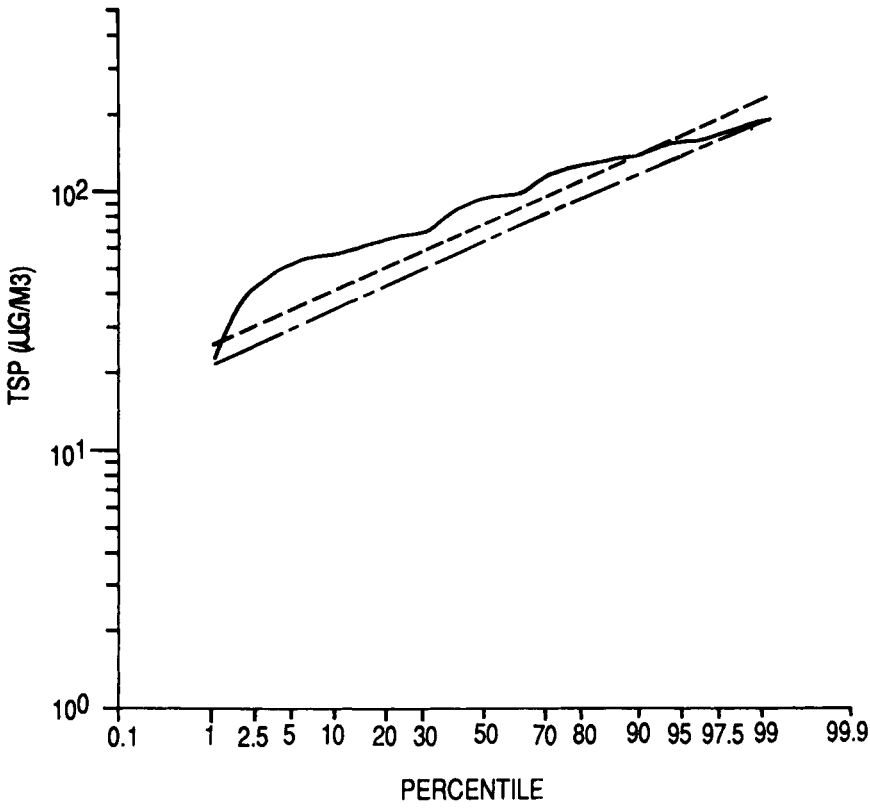


Fig. 2. Plot of predicted concentrations, using both Jamboree Heights (—·—) and ratio (- - - -) background corrections, compared with observed TSP (——) concentrations for Woolloongabba, Queensland, Australia, 1978-1979 (Simpson *et al.*, 1987).

times and locations than those measured. For example, relaxing the requirement for time/space pairing in St Louis simulations reduced the bias from –32 percent to +4 percent (Seinfeld, 1988). Part of the difficulty in matching ozone maxima at the correct time and location is due to the inherent difficulties in reconstructing the meteorological and emissions fields on the day in question. Seinfeld (1988) concludes that grid-based photochemical air quality models with up-to-date chemistry, wind-field treatment, and numerical techniques have reached a level of accuracy that may be difficult to improve upon in the near future.

The most important application of the photochemical models is in predicting the consequences of various smog control policies. The approach adopted, in part because of these model predictions, is mainly to control the emissions of hydrocarbon precursors and not $NO_x$ (e.g. see Chock and Heuss, 1987). However, it is by no

means clear that this approach is working (e.g. see Lindsay *et al.*, 1989). Given the rising $NO_x$ levels in all industrialised countries, this gives some cause for alarm and perhaps a re-examination of the control approaches being adopted.

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