THE EVALUATION OF PREDICTIVE TECHNIQUES TO DETERMINE CONCENTRATION LEVELS OF ATMOSPHERIC POLLUTANTS IN PRETORIA

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OPSOMMING:

Daar bestaan 'n aantal deskundige modelle vir die beskrywing van die despersie van besoedelstowwe vanuit 'n veelfout van bronne in 'n stad. 'n Gaussiese pluim en twee eenvoudige modelle is in die modelstad Pretoria toegepas en ge-evalueer. Voorspellings van maandelikse, seisoens en jaarlikse konsentrasievlakke van atmosferiese SO_2 is vergelyk met waarnemings. Dit is bevind dat die eenvoudige net-model onrealistiese resultate lewer. Toepassing van 'n Gaussiese pluim en die *(Cq/u)* model as basis vir effektiewe beheer van stedelike lubesoeding deur die owerhede word bespreek en kritiese model parameters word uitgeken.

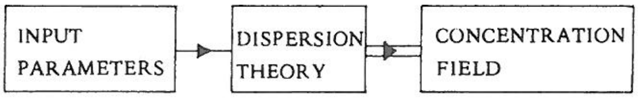
SYNOPSIS:

Several mathematical models are available to describe the dispersion of multiple pollutant emissions into the urban atmosphere. A Guassian plume model and two simple models are implemented and evaluated using Pretoria as a model city. Predictions of monthly, seasonal and annual concentration levels of atmospheric sulphur dioxide are compared with observations. The simple grid model is found to give unrealistic results. The applicability of the Gaussian plume model and the *(Cq/u)* model as a basis for the effective control of urban air pollution by control authorities is discussed and critical parameters of the models are identified.

INTRODUCTION

The rapid economic development of South Africa in recent decades resulted in the need for introducting measures designed to control the increasing air pollution problem. When a development project is to be commenced, with new industries and new residential zones, it is not possible to carry out intelligent planning of the development project unless the effect of an emission at a given point can be equated with the production of the pollutant concentration at a point of social concern. The nature, distribution and intensity of pollutant emission, the changing dispersive and removal capacity of the polluted atmospheric layer and the effect of the city on this capacity can be recognized as the main aspects of the dynamic relationship between a city and its atmospheric environment. Thus, the mathematical description of the physical processes which govern the travel of pollutants from their point of origin to sensitive parts of the urban area has become of considerable importance.

The exact description of the dispersion process is aggravated by the intractability of the basic equation derived for the atmosphere from the principles of conservation of mass, momentum and energy. To alleviate the problem of mathematical formulation, several approaches have been proposed in which a varying degree of idealization is introduced to solve or to re-state the basic equations. As a result of the idealization approximate solutions are available which in turn provide the basis for the applied models of pollutant dispersion form multiple sources. The logical structure of a model is shown in Figure 1. Whereas the dispersion theory aims at a solution applicable to any region of interest, the model input parameters are used to characterize one particular region and the state of the atmosphere for each individual application. The result of the mathematical simula-



MODEL INPUT PARAMETERS

- EMISSION INVENTORY
- METEOROLOGICAL PARAMETERS
- GEOGRAPHICAL PARAMETERS
- LONG-RANGE TRANSPORT OF POLLUTANTS
- REMOVAL PROCESSES

WORKING THEORIES OF POLLUTANT DISPERSION

- STATISTICAL (GAUSSIAN) THEORY
- GRADIENT TRANSPORT THEORY
- SIMILARITY THEORY
- SIMPLE DETERMINISTIC AND EMPIRICAL MODELS

AREAS OF APPLICATION

- TOWN PLANNING SCHEMES
- SITING OF INDUSTRIES
- WARNING SYSTEM FOR POLLUTION EPISODES
- VALIDATION OF MODELS
- FURTHER RESEARCH AND DEVELOPMENT

FIG 1 *The logical structure of an air pollution dispersion model* tion is a predicted concentration field of the pollutant under consideration. Predictions of long-term concentration levels may be used as a guide for town planning schemes, development of new industries, etc. Predictions of short-term concentration levels may form a part of a warning system in cases of severe pollution episodes.

The degree of accuracy and the applicability of individual models vary considerably under differing conditions and no model is known to be superior to others in every respect. The performance of a model in a new area of application can often be determined only in the course of the application. When a model is implemented and evaluated in a real-world situation the parameters which are critical for its predictive ability can be identified. Based upon this identification, the accuracy of the model which has shown a satisfactory degree of realism, can further be improved, whereas an unsatisfactory model is rejected. In this paper the implementation and the evaluation of a Gaussian plume model and two simple models to predict the concentration of atmospheric sulphur dioxide in urban Pretoria are presented.

THE MODELS

The Gaussian plume model

The standard Gaussian plume formula [1,2] is used to describe the distribution of pollutant concentration from *isolated (point) sources)* in the urban area. If a composite frequency function *f (i, j, k)* is described as the frequency with which the pollutants are transported toward the receptor from the *i-th* class under vertical dispersion conditions represented by the stability class *k*, the concentration at the receptor *(x, 0, 0)* is calculated as

$$\chi(x,0,0) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{1}{2\pi}\right) \sum_{m=1}^{M} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{Q_m \quad f(i_m, j, k)}{r_m \cdot u(j) \cdot \sigma_z(r_m, k)} \exp \cdot \left(\frac{H_m^2}{2\sigma_z^2(r_m, k)}\right) \qquad \ldots\ldots\ldots (1)$$

where the subscript *m* refers to individual sources situated at the distance *r* from the receptor. Q is the rate with which the pollutant is emitted at the height *H* above the ground and the symbol σ_z parameterizes the vertical dispersion of the pollutant cloud along the path of its travel.

The density and nature of emisions in certain parts of the urban area make an individual assessment of all sources unpractical and prohibitive in terms of computer time. Instead, *area sources* are defined on a horizontal grid of simple geometrey as the total amount of pollutants emitted from the area elements. The expression for calculating the contribution of area scources to a receptor point at the ground level may be derived in a form similar to Equation (1) in which the point source strength Q is replaced by the total emission rate from the area element.

The simple models

In simple models the emphasis is on a relatively simple calculation which can often be performed without the use of a large computer. This aim is achieved by making simplifying assumptions concerning the physical basis of the dispersion process.[3,4]

In the *grid model*[5] the concentration in the receptor square to upwind area sources is calculated as

$$\chi = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{\left(\frac{\Delta x}{2}\right)^{1-b}}{ua\,(1-b)} \left\{ q_o + \sum_{i=1}^{N} q_i \left[(2i+1)^{1-b} - (2i-1)^{1-b} \right] \right\} \qquad \ldots\ldots.(2)$$

where q_i is the area source strength in the *i-th* grid square and *N* is number of grid squares of side Δx between the receptor and the upwind edge of the modelled area. The concept of the grid model is illustrated in Figure 2. The contribution by the point sources to the total concentration value is obtained separately by using the Gaussian plume formula (Equation 1).

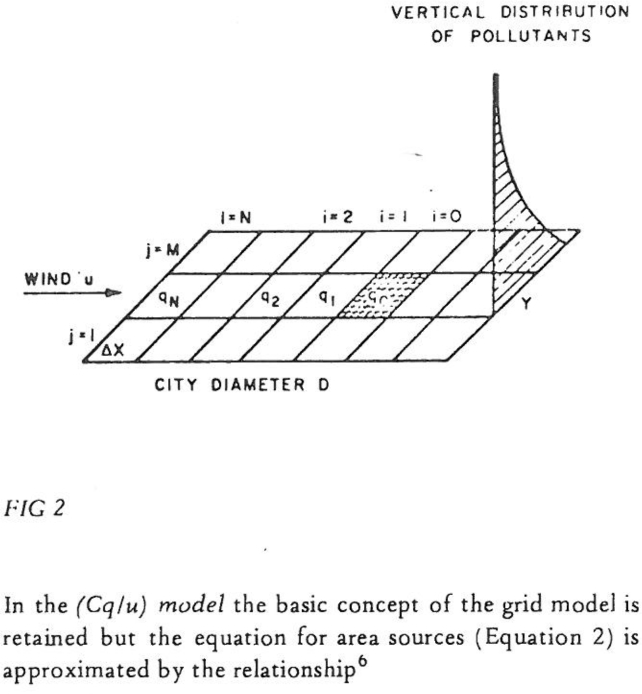


FIG 2

In the *(Cq/u) model* the basic concept of the grid model is retained but the equation for area sources (Equation 2) is approximated by the relationship[6]

$$\chi = C\,\frac{q_o}{u} \qquad \ldots(3)$$

in which the value of the factor *C* is allowd to vary with the degree of atmospheric stability.[7] The validity of the *(C q/u)* approximation for describing the mean distribution of pollutants from urban area sources has been confirmed by several workers.[8,9,10]

THE EVALUATION OF THE MODELS

In order to obtain the data base for the application of the models an experimental programme was carried out in Pretoria which included the monitoring of sulphur dioxide at various locations and a variety of meteorological observations. A detailed study of the SO_2 emission pattern was also completed for both the winter and summer seasons. The models were applied to obtain predictions of the mean concentration levels of atmospheric sulphur dioxide. The predictions which ranged from monthly to seasonal and annual estimates were compared with observations. The standard error of estimate, the mean deviation and the coefficient of correlation were used to measure the performance of each model as shown in Table 1.

In order to assess the relative importance of the model parameters a sensitivity analysis of the models was carried out. Random and systematic variations were introduced into the data input set and the responses of the models were studied. When the same rate of fractional change of the input parameters was introduced the variation of the vertical disperiosn parameter σ_z resulted in the largest digression in the predicted SO_2 concentration (See Figure 3). This high sensitivity to a systematic variation of the parameter σ_z was followed in magnitude by the sensitivity to variations of the emission rate and the wind speed.

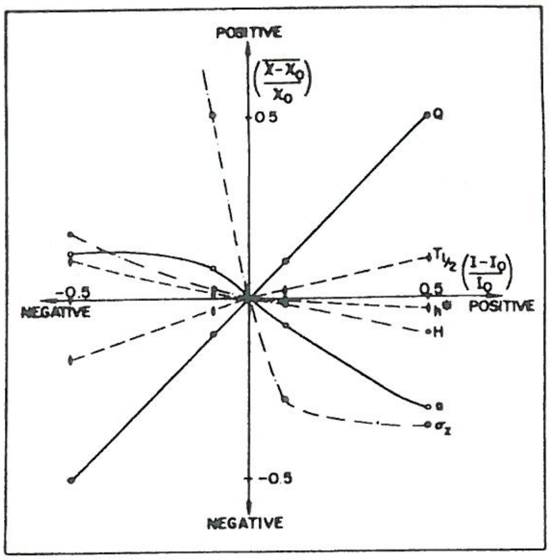


FIG. 3

TABLE 1 THE RESULTS OF THE CORRELATION BETWEEN MODEL PREDICTIONS AND OBSERVATIONS OF SO_2 CONCENTRATION LEVELS IN PETORIA

MODEL	MEASURE	PERIOD OF APPLICATION				
		1 Month (July 1977)	1 Month (Nov 1977)	3 Months (Winter 1977)	3 Months (Spring 1977)	6 Months (June–Nov 1977)
Gaussian plume model	Correlation coefficient	0,88	0,80	0,86	0,63	0,77
	Mean rel. deviation	– 0,15	– 0,26	– 0,09	+ 0,07	– 0,08
	Standard error	9,9 μg/m³	10,4 μg/m³	10,6 μg/m³	20,8 μg/m³	14,5 μg/m³
Grid model	Correlation coefficient	0,57	0,64	0,55	0,72	0,52
	Mean rel. deviation	+ 1,72	– 0,05	+ 1,50	– 0,02	+ 0,39
	Standard error	91,5 μg/m³	8,9 μg/m³	81,6 μg/m³	8,7 μg/m³	18,4 μg/m³
(Cq/u) model	Correlation coefficient	0,82	0,81	0,70	0,84	0,85
	Mean rel. deviation	+ 0,63	– 0,28	+ 0,46	– 0,23	+ 0,03
	Standard error	21,6 μg/m³	7,5 μg/m³	26,1 μg/m³	7,8 μg/m³	8,1 μg/m³

In addition to an analysis of the effect of single parameters on the performance of the Gaussian plume model, the sensitivity to possible errors in the determination of the composite frequentcy function *f(i, j, k)* was also investigate. Whereas random errors did not result in significant deviations in the predicted concentration levels, the situation changed considerably when systematic errors were introduced into the frequency function. When the stabiltiy class *k* was changed systematically by one category towards a more stable category (A→B, B→C, C→D, D→E, F) the mean deviation in the predicted concentration was + 24 % with individual values ranging from 9 to 100 % of the original concentration. A change towards a less table category produced a mean reduction of 8 % and a narrower range of deviations. Similarly, a systematic overestimation of the wind speed class *j* by one class (class 5→4, 4→3, 3→2, 2→1, 1) resulted in an increase in the concentration of + 12,5 %. The corresponding reduction in the concentration for a positive error in the speed classification by one class was − 40 %. In both cases the individual deviations ranged from 0 to 100 % of the original value. A systematic error of 22,5° in the determination of the mean wind direction did not produce a significant mean deviation of prediction results. More significantly, however, the range of the deviations at individual receptors was extremely wide and covered an interval of − 75 % to + 100 %.

DISCUSSION

The application of the Gaussian plume model in Pretoria has shown that the model realistically reflects the spatial disposition of the main polluted areas during the various seasons of the year. Results of the correlation between the predicted concentrations and observations have not indicated any major deviations which would necessitate a basic revision of the model. A realistic reflection of the spatial concentration distribution and a fair correlation between concentration predictions and observations in general cannot, however, be interpreted as proof of the model's capability to simulate pollution levels at all locations within the area with the same degree of accuracy. Owing to an interaction of topographical and meteorogical factors such as the development of local gravity flows under low-wind conditions at night, especially in winter, and the sheltering effect of the ridges, local modifications of dispersion conditions frequently occur.[11] Although the nature of long-term modelling applications tends to have a smoothing effect on the principally short-term modifications, the resulting variations of the wind and stability fields can be expected to cause local deviations from the predicted concentration field.

The application of the grid model has indicated that the model does not adequately describe the dispersion process in Pretoira. A significant overprediction by a factor of three to four was consistently found during the winter season (see Table 1). The predictions for the industrial part of the city where elevated point sources predominate agreed considerably better with the observations than the predictions for the city centre where a large number of low-level sources are situated. In winter most of the low-level sources are active during the times of the day which are associated with the development of strong surface-based inversions under low-wind conditions. The surface-based inversions are most intense in a shallow layer immediately above the ground, and the height at which the effluent is released plays a vital role in the dispersion process. In contrast to that situation, all area sources in the model are assumed to be situated on the ground. Although the concept of defining a spatially invariable mean wind vector for the entire area and the absence of the removal of airborne pollutants from the atmosphere in the model equation may also contribute to the reduced performance of the model, the assumption of effluent release at ground-level must be seen as the major cause of its failure.

When the treatment of the area sources is replaced in the grid model by the *(Cq/u)* approximation it is necessary to determine the value of the stability-dependent factor *C*. In order to obtain predictions for periods of distinct stability conditions by the model the seasonal variability of the factor *C* was determined experimentally.[7] The *(Cq/u)* model has been shown to yield results with a degree of realism comparable to the results of the complex Gaussian plume model.

CONCLUSIONS

A Gaussian plume model and two simple models were applied to obtain predictions of monthly, seasonal and annual mean concentration levels of atmospheric sulphur dioxide for Pretoria. Whereas the Gaussian plume model and the simple *(Cq/u)* model realistically reflected the levels and the distribution of air pollution, the grid model failed to simulate the production of the pollutant concentration with the same degree of realism. The Gaussian plume model and the *(Cq/u)* model differ in the degree of complexity, the requirements on the amount and quality of the input data and in the detail of the resulting information. Thus, the application of the models by control authorities concerned with pollutant emissions in urban areas will depend on a number of factors.

In order to apply the Gaussian plume model effectively, an extensive data collection programme and the use of a large computer installation are required. The accuracy and the detail of the results are determined by the quality of the critical input parameters such as the wind and stability fields, the vertical dispersion parameter σ_z and the emission rate. Whereas a random error in the critical set of input data does not cause a significant error in the overall performance of the model, systematic errors, even of a lesser magnitude, result in large deviations of the model predictions.

The simple *(Cq/u)* model can be applied with a comparable degree of realism provided that the variation of the stability-dependent factor *C* in the area of interest is known. It is an inexpensive and effective model, especially in applications where only a limited amount of input data can be made available.

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LEGEND TO FIGURES

FIGURE 2.

The concept of a grid model. The pollutants are emitted at ground level from (M x N) area sources of differing strength q_i and advected downwind by the mean wind speed u.

FIGURE 3.

The deviation of concentration predictions $\left(\frac{\chi - \chi_o}{\chi_o}\right)$ in response to systematic variation of input parameters $\left(\frac{I - I_0}{I_0}\right)$. The parameters are:

Q = emission rate
$T_{\frac{1}{2}}$ = pollutant half-life
h^* = mixing height
H = emission height
u = central wind speed
σ_z = vertical dispersion parameter