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# MODELLING THE DISPERSION OF AIRBORNE POLLUTANTS IN THE PRETORIA URBAN AREA

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A Thesis Submitted to the Faculty of Science, University of the Witwatersrand, Johannesburg for the Degree of Doctor of Philosophy

Johannesburg 1979

This is to declare that this thesis
is entirely my own work and has not
been previously submitted as a thesis
for any degree at any other university.

P. Zib

## ABSTRACT

The theory and methodology of urban air pollution dispersion models are reviewed to provide the background for a critical approach to modelling atmospheric pollution in South African conditions. It is shown that there is no evidence to suggest the existence of a universally applicable modelling technique. Three models of various degrees of complexity, the Gaussian plume model for multiple sources, the ATDL-grid model and the Gifford-Hanna simple model, are applied to predict long-term concentrations of atmospheric sulphur dioxide in the Pretoria urban area and evaluated against observations. Whereas the ATDL-grid model does not adequately simulate air pollution levels during the main pollution season in Pretoria, more realistic results are obtained by the Gaussian plume model for multiple sources and the Gifford-Hanna simple model.

The refinements introduced into the two models to further improve their performance are presented. A closer association between predicted and observed $SO_2$ concentrations is consistently obtained when an increasing number of wind and stability observations are used in the Gaussian plume model for multiple sources to simulate spatial variations in the dispersion conditions over Pretoria. The Gifford-Hanna simple model is refined by including estimates of hourly, monthly and seasonal air pollution concentrations. An objective weighting scheme is used in conjunction with experimental evidence to determine variations of the stability factor in the model. The methodology of future applications is discussed and it is shown that the refined Gifford-Hanna simple model provides a fast and inexpensive basis for predicting concentration levels of atmospheric pollutants from multiple sources with a degree of success comparable to the performance of the Gaussian plume model.

## PREFACE

The advancement of technology and a rapid urbanization in the recent decades have brought a new factor into the lives of many city dwellers - the polluted atmosphere. Air pollution meteorology, which deals with the capacity of the atmosphere to disperse man-made pollution, is receiving increasing attention from not only atmospheric scientists but also from the medical profession, environmentalists, industrialists, town planners and decision makers at all levels. A new field of scientific research, that of air pollution dispersion modelling, has been developed to describe the interaction between the emissions and the atmosphere in mathematical terms. Several problems, both theoretical and practical, have been encountered in attempts to design generally applicable dispersion models, thus bringing a degree of uncertainty into the utility of the mathematical description.

Two differing schools of thought exist at present with regard to modelling atmospheric dispersion. One approach deals with fundamental planetary boundary layer (PBL) modelling. The initial and boundary atmospheric conditions are established and continuously upgraded for use in a dispersion submodel to yield the concentration field of a given pollutant. PBL models are in an early stage of theoretical development and as such, at present, are unsuitable for routine applications. The same cannot be said of a variety of simplified air pollution dispersion models which have been developed in the USA and Europe and which form the basis of air pollution control programmes in many parts of the world. However, before these can be used in such programmes they need to be tested, validated and often modified for use in local conditions.

In South Africa, the problem of air pollution is compounded by the country's geographic position, climatological conditions and its coal-based economy. About 75 percent of South Africa's surface area is situated on a plateau at the altitude of above 1000 metres in the subtropical high pressure belt. The anticyclonic circulation, prevalent particularly in winter, results in a high frequency of strong atmospheric stability associated with

low wind speeds and generally low ventilation. The major part of the country's industries are located on the plateau where the necessary energy requirements are almost entirely derived from coal imposing a significant burden on the atmospheric resources. Immediately applicable dispersion models are required for the formulation of positive control policies in order to prevent a serious deterioration of the situation.

Despite the growing awareness among the scientific and industrial community, the operational use of mathematical models to relate the production of pollutant concentrations at points of social concern with emissions and specific atmospheric conditions in South Africa has been minimal. It is not even known at this stage whether the available dispersion models which had been developed and applied predominantly in mid-latitude industrial countries of America and Europe may be used with safety to describe dispersion in South African plateau conditions. Satisfactory answers must also be found to questions of exactly how the models must be applied, how accurate are their predictions and what can be done to improve their performance and accuracy. In order to meet the current need and for a meaningful application of routine predictive models, it is necessary for research to be carried out into the mathematical foundations, methodology and particularly the applicability of urban air pollution dispersion models.

In this thesis an attempt is made to determine the utility of mathematical modelling of atmospheric pollution in an urban area, that of Pretoria, and to provide the methodological basis for current dispersion modelling in South African conditions. More specifically the aims of the thesis are:

(i) to review existing models emphasising physical aspects and computer implementation of the models,

(ii) to apply certain models to the Pretoria urban area, and thereafter

(iii) to evaluate the models using a specifically designed experimental programme,

(iv) to reconcile the differences in the performance of models of varying degrees of complexity, and finally

(v) to refine the best-performance models for use in the Pretoria urban area.

The thesis is devoted, on the one hand, to the analysis of the general aspects of urban air pollution dispersion modelling, and on the other, to the application to specific South African conditions using

Pretoria as a model city. In presenting the work, it is divided into four parts. Part I gives an introduction, historical perspectives and presents the model elements. Part II considers the application of the Gaussian plume model, the ATDL-grid model and the Gifford-Hanna simple model to Pretoria data; the results of the application are presented and evaluated against observations of sulphur dioxide concentrations. Based upon the evaluation, refinements to the Gaussian plume model and the Gifford-Hanna simple model are proposed and implemented in Part III. The thesis is concluded and a summary of the findings is presented in Part IV.

In the course of the research much of the work has been published. Chapter 2 has been presented as a critical review paper in Environmental Studies (1977); a substantive portion of Chapter 4 has been published in the South African Journal of Science (1978); part of Chapter 4 appeared in the Journal of Applied Meteorology (1978) and a substantive portion of Chapter 5 has been presented in Proceedings: International Conference on Air Pollution (1979). Finally, papers based on parts of Chapter 6 have accepted for publication in the South African Journal of Science (1980) and in the Journal of Air Pollution Control Association (1980).

I wish to express my gratitude to my supervisors: Professor P.D. Tyson, the Director of the Climatology Research Group at the University of the Witwatersrand, Johannesburg for his constructive criticism and his guidance in the preparation of the final draft, and to Dr. G.P.N. Venter, the Head of the Air Pollution Research Group, Council for Scientific and Industrial Research (CSIR), Pretoria who first stimulated my interest in dispersion modelling and offered encouragement and general interest throughout the research.

Without the subtle support of my wife, Jana, and my daughter, Martina, the study would not have been possible and I wish to dedicate the thesis to them.

The study is a part of the cooperative Pretoria Mouel Project which was initiated in 1976 by the Air Pollution Research Group of the CSIR, Pretoria and the Climatology Research Group of the University of the Witwatersrand, Johannesburg. The experimental programme was funded by the CSIR through the National Programme for Environmental Sciences.

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## LIST OF SYMBOLS

An underbar indicates that the quantity is a vector.
An overbar indicates the mean value.
A prime indicates a fluctuation from the mean value.

### Roman symbols

| | |
|---|---|
| $a,b$ | Stability parameters in $\sigma_z(x) = ax^b$ |
| B | Parameter expressing the vertical distribution of pollutant concentration |
| $B_s$ | Weighting parameter |
| $b,c$ | Universal constants |
| C | Stability-dependent factor in $\chi = C \frac{q}{u}$ |
| $c_i$ | Coefficient of proportionality |
| $\underline{c}$ | Wind vector |
| $c_p$ | Specific heat at constant pressure |
| $c,d$ | Stability parameters in $\sigma_y(x) = cx^d$ |
| D | City diameter |
| $D_x$, $D_y$, $D_z$ | Diffusion term |
| d | Displacement length |
| E | Total emission rate from the urban area |
| F | Buoyancy term $\equiv \frac{g\, Q_h}{\pi \rho c_p T}$ or rate of transport (Ch.2) |
| $F_D$ | Deposition flux |
| $F_x$, $F_y$, $F_z$ | Advective term |
| f | Coriolis parameter |
| f(i,j,k) | Frequency function of occurence of variates i,j,k |
| f* | Flushing frequency |
| g | Gravitational constant |
| H | Effective stack height |
| $H_f$ | Heat flux |
| h | Physical stack height |
| $\Delta h$ | Plume rise |
| h* | Mixing height |
| I | Input variable |
| $K_T$ | Molecular heat conductivity |

| | |
|---|---|
| $K_x$, $K_y$, $K_z$ | Eddy diffusivity |
| k | von Karman constant |
| $k_s$ | Arbitrary constant (Ch.6) |
| L | Monin - Obukhov length $\equiv \frac{u_*^3 \rho c_p T}{k g H_f}$ |
| m,n,p,q,s | Empirical constants for power law |
| P | Meteorological variable |
| p | Atmospheric pressure |
| Q | Point source strength |
| $Q_h$ | Heat emission rate |
| q | Area source strength |
| R | Removal term |
| $R_j$ | Radiant heat term |
| $R_x$, $R_y$, $R_z$ | Correlation coefficient |
| Ri | Richardson number $\equiv \frac{g}{T} \frac{\partial \theta}{\partial z} \left(\frac{\partial u}{\partial z}\right)^{-2}$ |
| r | Distance between source and receptor |
| S | Solar radiation |
| $\hat{S}$ | Standard error of estimate |
| s | Stability parameter $\equiv \frac{g}{\theta} \frac{\partial \theta}{\partial z}$ |
| T | Temperature |
| $T_{\frac{1}{2}}$ | Half-life constant |
| t | Time |
| $t_L$ | Lagrangian time scale of turbulence |
| $\Delta t$ | Time interval |
| U | Bulk wind speed |
| u, v, w | Wind speed components |
| $u_*$ | Friction velocity $\equiv \left(\frac{\tau}{\rho}\right)^{1/2}$ |
| V | Volume of air |
| $v_D$ | Deposition velocity |
| $W_s$ | Weighting factor |
| X | Predicted value |
| x, y, z | Cartesian coordinates |
| $\Delta x$ | Grid size |
| Y | Observed value |
| $z_o$ | Surface roughness length |

Greek symbols

| | |
|---|---|
| $\alpha$ | Constant of proportionality |

| | |
|---|---|
| $\beta$ | Ratio between Lagrangian and Eulerian time scales or empirical constant for power law (Ch.3) |
| $\Gamma$ | Gamma function |
| $\gamma$ | Stability ratio |
| $\delta$ | Kronecker delta |
| $\delta_m$ | Parameter relating pollutant concentration to mixing height |
| $\epsilon_{i,j,k}$ | Alternating tensor |
| $\underline{n}$ | Unit vector parallel to the earth's axis of rotation |
| $\theta$ | Potential temperature |
| $\lambda$ | Removal rate |
| $\mu$ | Dynamic viscosity |
| $\nu$ | Kinematic viscosity |
| $\xi$ | Lagrangian time |
| $\xi, \eta, \zeta$ | Lagrangian coordinates |
| $\rho$ | Atmospheric density |
| $\sigma_x, \sigma_y, \sigma_z$ | Standard deviation of concentration distribution |
| $\tau$ | Shearing stress or time interval (Ch.6) |
| $\phi$ | Angle |
| $\phi_m$ | Monin - Obukhov universal function |
| $\chi$ | Concentration of pollutants in air volume |
| $\Omega$ | Angular frequency of the earth's rotation |

# PART I - MODEL ELEMENTS

# CHAPTER 1

## INTRODUCTION AND BACKGROUND

### 1.1 The problem

In an urban area a variety of pollutants are released from a large number of sources into the lower layer of the atmosphere. The sources vary in the emission rate, the height of release and the pattern of release according to the nature of the pollutant-generating operations. Besides a relatively small number of large sources such as power-generating plants and major industrial complexes, a large number of activities that result in increasingly polluted city air are to be found in urban areas. Light industrial and commercial activities, space heating in business and residential areas as well as the transportation of goods and people are among the most frequent contributors to the air pollution problem.

The pollutants advected downwind from emission sources by the prevailing wind are dispersed vertically and horizontally by the turbulent action of the atmosphere. The degree of advection and dispersion is determined by the physical properties of the planetary boundary layer present over the urban area at any given time. The assessment of the state of the planetary boundary layer particularly wind speed, wind direction and atmospheric stability, and of the changes that continuously take place in the layer constitutes an important part of air pollution studies.

As the rural air passes over the urban area its physical properties are modified by the city itself. Two of the main factors causing the modification are an increase in surface roughness and a change in the heat budget. The increase in surface roughness due to buildings, tall constructions, etc. often results in a decrease of the wind speed and also affects the direction of the air flow and its turbulence characteristics (Zib and Halliday, 1978). The change in the heat balance is caused not only by direct releases of anthropogenic heat, but also by the changed

characteristics of the surface. In the presence of large vertical surfaces and materials such as concrete, bricks and tarmac, more solar energy is absorbed and stored in a city than in a rural area during the day. This heat is released back into the atmosphere when the radiation flux is reversed at sunset. As a result, the temperature in a city is expected to exceed the temperature outside the complex (Bornstein, 1968, Tyson et al., 1973, Gutman and Torrance, 1975). Both the atmospheric instability and mixing height also experience a positive change.

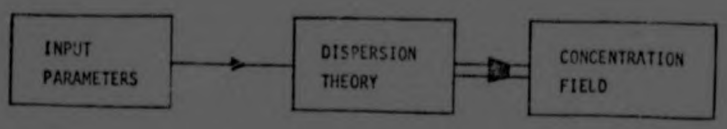
In addition to advection and dispersion, the density and distribution of airborne pollutants is controlled by a number of removal and transformation processes. These processes act towards a decrease in the actual concentration of the pollutant species by removing it from the polluted atmospheric layer or by transforming it into a different chemical substance. Depending on the chemical nature of the pollutant, the transformation may take place in the atmosphere or on the ground where the pollutant has been deposited.

## 1.2 The structure of a model

The logical structure of an air pollution dispersion model is shown in Figure 1.1. A mathematical expression which describes the effects of the atmosphere on the behaviour of pollutants is the central element of the model. Several working theories of pollutant dispersion may be used to derive the mathematical expression.

Several boundary conditions have to be specified concerning the emissions, meteorology and atmospheric chemistry in the urban area to which the model is to be applied. The main input parameters which are normally required by a dispersion model are listed in Figure 1.1.

The result of the mathematical simulation is a predicted concentration field of the required temporal and spatial resolution. The resulting information on the distribution of a specific air pollutant can be used for both practical and research purposes. Predictions of long-term concentration levels often serve as a guide for town planning schemes, development and siting of new industries, etc. Predictions of short-term concentration levels may form a part of a warning system in cases of




MODEL INPUT PARAMETERS

- EMISSION INVENTORY
- METEOROLOGICAL PARAMETERS
- GEOGRAPHICAL PARAMETERS
- 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

Figure 1.1 The logical structure of an air pollution dispersion model

severe pollution episodes. Generally, all regulations and policies with regard to air pollution may be tested on a model before they are applied in practice. In research applications models which have been evaluated using an analysis of the observed and predicted concentrations may be refined or re-developed. In the course of the evaluation a better understanding of the physical and chemical aspects of urban air pollution is often gained.

## 1.3 Some historical perspectives

The process of dispersion of pollutants emitted from individual elevated sources such as the tall stacks of fossil fuel-burning, power-generating plants has long been subjected to investigation. An account of the early work is given by Sutton (1953). While the problem of dispersion from individual sources was receiving continuous attention, the survey of atmospheric pollution in the city of Leicester, U.K. (DSIR, 1945) remained an isolated attempt to study the concentration distribution of pollutants from multiple urban sources. The first urban air pollution dispersion models were described in the late 1950's by Frenkiel (1956), Lucas (1958) and Leavitt (1960). A more consolidated approach to the air pollution problem in urban areas was initiated at the symposium 'Air over Cities' in 1961. In his opening address to that symposium, Stern (U.S. Department of Health, Education and Welfare, 1961) predicted the development of urban air pollution modelling as follows:

> 'The electronic computer will develop local forecasts of air quality and the maximum source strength distribution that will keep pollutant emissions within air quality standard limits ... By 1985 ... we will be giving quotas to the highway entrance control points as to the number of vehicles permitted to pass each hour, and to industrial sources for their hourly emission quotas. Also we will determine which portion of energy used in household and commercial enterprises is to be drawn hourly from energy storage reserves maintained for that purpose and which portion may come from new energy conversion processes. Thus on bad days we will balance the ability of the atmosphere to handle the pollution with the amount that we throw into the atmosphere.
>
> About at this point the computer will be hooked up to the telemetered local air quality monitoring network to make hourly comparisons between the predicted and the actual concentrations and to prepare hourly amendments to the source strength quotas.'

Following this initial period in the development of simulation techniques for urban air pollution, the decade from 1960 to 1970 has been characterized by the increasing use of the Gaussian dispersion model for multiple sources. Its applications may be found in papers by Pooler (1961), Clarke (1964), Turner (1964), Koogler et al.(1967), and Miller and Holzworth (1967). In summing up a symposium on multiple-source urban dispersion models nine years later, Stern (1970) looked back at the development of mathematical modelling by saying:

> '... models serve to test our understanding of the physical nature of the atmosphere and the sources we are modelling. If we can't model it, we don't understand it. A decade ago, we tended to say that we understood these phenomena, but lacked the programming, computational, and statistical capabilities to resolve the problem. Today, the tables are turned; we have programming, computational, and statistical capability far beyond our needs, but lack the physical inputs and concepts to fully exploit these capabilities ...'

Apart from stressing the importance of physical understanding of the problem, the symposium on multiple-source urban dispersion models in 1970 has also marked the beginning of polarization between models for practical use and models for research applications. After 1970 the Gaussian plume model in its original form remained the most frequently employed approach to practical problems and in addition many simple models have also been developed. The box model (Lettau, 1970), the ATDL model (Gifford and Hanna, 1970, Hanna, 1971, Gifford and Hanna, 1973) and non-deterministic models based upon the regression analysis between the pollutant concentration and selected parameters (Barth, 1970, Smith and Jeffrey, 1972, De Nevers and Morris, 1975, Mc Collister and Wilson, 1975) are the best known examples of the simple techniques.

The necessity to incorporate the simulation of kinetic reactions of chemically reactive pollutants on the other hand resulted in a marked trend towards the development of another category of models based upon the gradient transport theory of turbulent flows in the early 1970's. Attempts to solve the diffusion equation numerically and so evade the constraints placed on the analytical solutions have been facilitated by the concurrent development of new techniques for numerical integration of partial differential equations using large computer installations.

Most recently, increasing attention is being given to the complete set of equations derived from the principle of conservation of mass, momentum and energy in the planetary boundary layer. Analytically intractable because of the closure problem, this set of equations in the form of the Boussinesq approximation provides a working basis for attempts to overcome the closure problem by modelling higher-order terms empirically and solving the equations numerically.

Generally, all models represent approximate solutions in which a certain degree of idealization of the dispersion process has been introduced in order to obtain working estimates of atmospheric pollution levels. The applicability of existing models is restricted by the ability of the theoretical approach adopted in a particular model to represent the true physical processes in the atmosphere. The reliability of existing models is further influenced by the accuracy and representativeness of a wide range of meteorological, geographical and emission parameters used as input information for the calculational schemes.

# CHAPTER 2

## THEORY OF URBAN AIR POLLUTION DISPERSION MODELS

### 2.1 General considerations

A full description of pollutant dispersion in the planetary boundary layer can only follow from an understanding of the physical processes governing turbulent flow in the atmosphere. Generally, a set of equations is derived for turbulent flows (Landau and Lifschitz, 1959) from the principles of:

(i) conservation of mass (the continuity equation),

(ii) conservation of momentum (the Navier-Stokes equations), and

(iii) conservation of energy (the entropy equation and the equation of state).

This set of equations is intractable in its general form due to the non-linearity of the Navier-Stokes equations. In numerous investigations of turbulent flows a set of approximate equations, the so-called Boussinesq approximation (Chandrasekhar, 1961), has been used instead. The approximation involves the assumptions that:

(i) the variations of temperature-dependent density only become significant in gravity terms,

(ii) the dynamic viscosity and the molecular heat conductivity remain constant,

(iii) the convection is shallow, and

(iv) the temperature of the fluid is changed by the flux of heat only, no heat is generated by viscous stresses.

The Boussinesq equations consist of six equations (Busch, 1973)in

which the symbols p,T,ρ denote the variable static pressure, temperature and density of the atmosphere, whereas the same symbols with the subscript 0 refer to a reference state. The physical properties of the flow are further described by the dynamic viscosity μ, specific heat at constant pressure $c_p$ and molecular heat conductivity $K_T$. The velocity components $u_i$ (i=1,2,3) of the flow are expressed in a Cartesian coordinate system rotating with the earth, where the x - axis is orientated in the direction of the mean surface flow. The Coriolis acceleration is expressed in terms of the angular frequency of the rotation of the earth Ω and the unit vector $n_j$ which is parallel to the axis of rotation. Following the Einstein summation convention the principle of conservation of mass is expressed by the continuity equation

$$\frac{\partial u_i}{\partial x_i} = 0 \qquad (2.1)$$

The conservation of momentum is decribed by the three-component momentum equation

$$\rho_o \frac{du_i}{dt} = -\frac{\partial(p-p_o)}{\partial x_i} + \rho_o g \frac{(T-T_o)}{T_o} \delta_{3i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} - 2\rho_o \Omega \varepsilon_{ijk} n_j u_k \qquad (2.2)$$

which states that the rate of increase of the momentum must be in balance with the forces acting upon the fluid. The forces as represented by the right-hand side of Equation (2.2) are the pressure force, the buoyancy and viscous force and the Coriolis force.

The conservation of energy is expressed by the thermodynamic energy equation and the equation of state. In the entropy equation

$$c_p \rho_o \frac{d(T-T_o)}{dt} = c_p \rho_o K_T \frac{\partial^2 (T-T_o)}{\partial x_j \partial x_j} - \frac{\partial R_j}{\partial x_j} \qquad (2.3)$$

the rate of increase of the fluid temperature is due to changes in the molecular heat conductivity and the radiant heat transfer respectively. The equation of state

$$\frac{\rho-\rho_o}{\rho_o} = -\frac{(T-T_o)}{T_o} \qquad (2.4)$$

which expresses the two variables that define the state of the fluid completes the set.

Equations (2.1 - 2.4) represent an open system in which there are more unknowns than equations and therefore more equations are needed to close the system. The set of equations can be closed and a solution obtained when the higher-order terms are expressed empirically. Although obtainable in principle, the solutions of Equations (2.1 - 2.4) depend on the selection of adequate empirical expressions for the higher-order terms. In many instances, interim results have to be evaluated against experimental data in order to contain the deviations within acceptable limits or to determine the numerical values of empirical parameters. Initial applications of the second-order closure technique to problems in the atmospheric boundary layer have been reported by Donaldson and Hilst (1972), Deardorff (1972), Zeman and Lumley (1976,1978) and Lumley (1978). In the second-order closure, the second-order terms are retained and the third-order terms are modelled. While demonstrating the potential of the empirical closure of the equations for the atmosphere, the results have indicated that a general use of the technique is not possible at this stage of the development. Several aspects of the empirical closure will have to be studied and clarified before it can be applied to routine dispersion studies of air pollution.

In order to overcome the problem of mathematical formulation and to obtain practical solutions in the form of a model, several working theories have been proposed in which a varying degree of idealization is introduced to solve or to approximate the basic atmospheric equations. The dispersion models of urban air pollution are usually based upon one of the working theories that can be recognized as:

(i) the similarity theory,

(ii) the statistical theory, and

(iii) the gradient transport theory.

In addition to the basic theoretical treatment of dispersion, individual types of models are characterized by a number of other factors

which can be listed as follows:

- the theoretical basis for the treatment of dispersion,
- the physical assumptions made in the model,
- the applicability of the model to a specific area and the limitations of use,
- the input data requirements,
- the computational effort involved, and
- the degree of spatial and temporal resolution of the results.

In order to facilitate the selection of the best applicable modelling approach and to ensure realistic application of the model in a new area, the main features of the models as listed above have to be examined for each category of models.

## 2.2 Simple deterministic and empirical models

In simple models attempts are always made to ensure that calculations can be performed without the use of large computers. The simple models may be derived using either deterministic or empirical techniques.

### 2.2.1 Regression models

The regression models are based on a statistical analysis of observations obtained from one or a number of monitoring stations in the urban area. The relationship between concentrations of pollutants and significant emission and meteorological parameters is used for estimates of concentration levels at the specific locality.

2.2.1.1 Proportional models

Proportional models are the simplest type of models (Barth, 1970, De Nevers and Morris, 1975) and express the pollution concentration at a receptor in an area as proportional to total emissions in that area, viz.

$$\chi_i = C_i \cdot E \qquad (2.5)$$

where $C_i$ is the coefficient of proportionality for each receptor and E is the total emission rate for a given area. The effect of pollutants released from sources outside the receptor area may be included in the form of background concentration, that is, the concentration at the receptor prior to the introduction of local sources. Then the final concentration is calculated as the sum of the background concentration and the concentration due to emissions in the receptor area

$$\chi_i = \chi_{background} + C_i \cdot E \qquad (2.6)$$

The basic physical assumption of the proportional model that the concentration at a certain point is a function of the total emission rate only, excludes any further physical considerations. Thus the effect of the height at which the pollutant is released and the state of the atmosphere (degree of stability, wind speed, wind direction, etc.) are not considered. Also, the concept of background concentration as the contribution to the receptor from distant sources is difficult to apply in practice. It is not realistic to assume that the concentration measured at the receptor at any time will be the background concentration only, without any contribution from the local sources.

The proportional model gives a quick and approximate answer to practical problems where changes in the emission rate are the main consideration. If any meteorological parameter must be considered to be a variable, this model cannot be used.

2.2.1.2 Empirical models

Empirical models are based on the relationship between observed meteorological parameters and pollutant concentrations at a specific locality. The meteorological parameters chosen for correlation with observed values of pollutant concentration are those assumed to have a significant effect on the concentration pattern. If a significant relationship between one or more variables and observed values of concentration can be established, this may be used for further predictions. Only variations of parameters that were included in the original analysis can be considered for the predictions. Smith and Jeffrey (1972) estimated the daily average $SO_2$ concentrations in London by using the equation

$$\chi = 0{,}085 \cdot \left(1 + \frac{\delta_m}{6}\right) \left(1 - \frac{T - t}{28}\right) \left(5\overline{\chi} + 4\chi_p\right) + 0{,}15\overline{\chi} \quad (2.7)$$

where T is the minimum daily temperature in degrees Celsius, t is the number of hours per day during which the mean wind speed was below 6 kilometres per hour, and $\overline{\chi}$ and $\chi_p$ denote the mean and the previous levels of $SO_2$ concentrations. The parameter $\delta_m$ relates the concentration to the depth of the mixing layer. No value is assigned to $\delta_m$ for good vertical mixing. With a decrease in the mixing depth, the parameter $\delta_m$ increases to a maximum value of unity for very stable conditions.

Another model of this type was used by Bruntz et al. (1974) for estimates of maximum ozone concentrations in New York City. Solar radiation S in langleys, mean wind speed u in miles per hour and a maximum daily temperature T in degrees Fahrenheit were the parameters in the regression analysis and for the subsequent predictions of daily concentrations. The following equation was used:

$$\log (O_3 + 5) = -3{,}29 + 0{,}2 \log S - 0{,}61 \log u + 2{,}65 \log T \quad (2.8)$$

Similar developments have been reported by Peterson (1970) and McCollister and Wilson (1975). The analysis of observations

from a specific locality only reveals the relationship between variables and the concentration levels at this specific locality. A general application of the empirical model to other urban areas is not possible, since variables other than those considered originally may become significant. For example, Equation (2.7) does not consider changes in $SO_2$ emissions and so it is obvious that at a locality where the variations of emissions are pronounced, Equation (2.7) cannot be applied with success. For these reasons empirical models are best suitable for solving local pollution problems and also, where such a model has been developed, for testing other models applied to the same area.

### 2.2.2 Simple deterministic models

In contrast to empirical models deterministic models represent an attempt to describe the process of dispersion of pollutants in the urban atmosphere mathematically rather than statistically. The models are based on a greatly simplified approach to the physical aspect of the urban air pollution problem and aim at an analytical solution that can be obtained without the need to use a high-speed computer.

#### 2.2.2.1 The box model

If $\underline{c} = \underline{u} + \underline{v} + \underline{w}$ is the wind vector, Q is the source strength of pollutant release and $\chi = \chi\,(x,y,z,t)$ denotes the concentration of the pollutant, then the conservation principle yields

$$\frac{\partial \chi}{\partial t} + \nabla \underline{c} \cdot \chi - \nu \cdot \nabla^2 \chi = Q \qquad (2.9)$$

The physical meaning of Equation (2.9) is that a change in the concentration distribution is caused by one or a combination of the following processes:

(i) transport,

(ii) molecular diffusion,

(iii) emission rate.

Introducing mean and instant values $\chi = \bar{\chi} + \chi'$ (Reynolds decomposition) and time averaging transforms Equation (2.9) into

$$\frac{\partial \chi}{\partial t} + \bar{v} \cdot \bar{\chi} + \nabla \overline{v'\chi'} - \nu \nabla^2 \bar{\chi} = \bar{Q} \qquad (2.10)$$

where $\chi$ is the local concentration at a point in the area. The second and third terms on the left describe the transport by the mean motion and eddy fluxes respectively and the fourth term accounts for the molecular diffusion. In Lettau's model (Lettau, 1970) the mean transport in the vertical is considered negligible in relation to the vertical eddy flux ($\bar{\omega}\bar{\chi} \ll \overline{\omega'\chi'}$). In the horizontal the transport by the mean wind is considered dominant and both the horizontal eddy flux and the molecular diffusion are neglected. Since

$$\overline{u'\chi'} + \overline{v'\chi'} + \nu\nabla^2 \bar{\chi} \ll \overline{u\chi} + \overline{v\chi}$$

Equation (2.10) consequently reduces to

$$\frac{\partial \chi}{\partial t} + \frac{\partial(\overline{u\chi})}{\partial x} + \frac{\partial(\overline{v\chi})}{\partial y} + \frac{\partial(\overline{w'\chi'})}{\partial z} = \bar{Q} \qquad (2.11)$$

Subsequent assumptions made by Lettau (1970) concern the area source distribution, the thickness of the layer through which the pollutants are distributed over a city and the kind of distribution. Temporal variations of area source intensity are assumed and the uniform area source strength $q(t)$ over the whole urban area is defined as

$$q(t) = Q \cdot h^* + (\overline{w'\chi'})_{z=0} \qquad (2.12)$$

If a bulk wind speed $U(t)$ is defined as

$$U(t) = \frac{D}{\chi^*(t)} \left[ \frac{\partial \bar{u} \cdot \chi^*(t)}{\partial x} + \frac{\partial \bar{v} \cdot \chi^*(t)}{\partial y} \right] \qquad (2.13)$$

and a frequency $f^*$ as

$$f^* = \frac{U(t)}{D} + \frac{1}{h^* \chi^*(t)} \cdot (\overline{w'\chi'})_{z = h^*} \qquad (2.14)$$

where D is the city diameter and $\chi^*(t)$ is pollutant concentration uniformly distributed in the city air volume, Equation (2.11) becomes

$$\frac{\partial \chi^*(t)}{\partial t} + f^* \chi^*(t) = \frac{q(t)}{h^*} \qquad (2.15)$$

In the box model Equation (2.15) is applied to a one-dimensional problem under steady-state conditions, viz.

$$\bar{\chi}^* = \frac{q}{h^* f^*} = \frac{qD}{h^* \bar{u}} \qquad (2.16)$$

The first assumption that must be satisfied before Equation (2.16) can be used is the even distribution and uniformity of the sources in the area of application. The distance downwind at which a uniform vertical distribution of concentration will be reached under given meteorological conditions may be estimated by the method suggested by Turner (1969). When the concentration at the base of the stable layer that is situated at height h* above the centreline of the plume reaches one-tenth of the plume centreline concentration at the same distance downwind, the Gaussian vertical distribution begins to be affected by the restrictive layer. The distance $x_L$ is calculated from

$$h^* = 2{,}15 \ \sigma_z(x_L) \qquad (2.17)$$

where $\sigma_z(x)$ is the standard deviation of the Gaussian concentration distribution in the vertical. For a slightly unstable atmosphere and a constant mixing height of 500 m, both typical for an urban area (Holzworth, 1967), $x_L$ is 4 [illegible]. Turner further allows a transition period of the same length for the concentration to become uniformly distributed throughout the height of the mixing layer. Thus, the basic assumption of Lettau's model will be met at the distance of 9 km from the upwind edge and further downwind for slightly unstable conditions. Recent studies of the urban atmosphere (Tyson et al., 1973, Gutman and Torrance, 1975) indicate a rise in

mixing heights over large cities due to increased surface roughness and release of heat. With increasing mixing height, the distance downwind from which a uniform vertical distribution of concentration may be assumed will also increase.

2.2.2.2 The ATDL model

Gifford and Hanna (1970, 1973, 1975), Gifford (1972, 1973, 1974), Hanna (1971, 1973, 1977) at the Atmospheric Turbulence and Diffusion Laboratory (ATDL), National Oceanic and Atmospheric Administration (NOAA), developed an analytical model of the dispersion processes in an urban area. All large individual sources within the area (such as power plants, large industries with tall stacks etc.) are considered separately and their contribution is calculated using the standard Gaussian plume formula

$$X = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \cdot \frac{f\,Q}{\sigma_z\, r u \left(\frac{2\pi}{16}\right)} \cdot \exp\left(-\frac{H^2}{2\sigma_z{}^2}\right) \qquad (2.18)$$

A constant wind speed u and a wind direction frequency distribution f for 16 sectors are used. The pollution is emitted at strength Q at the effective height H and the distance r from the receptor. The effective height of release H is calculated as a sum of the physical stack height h and the rise of hot plume due to buoyancy forces $\Delta h$.

A multitude of lesser industrial, commercial and residential sources are combined and defined on a grid system as area sources. The mathematical basis is the simplified steady-state diffusion equation for two-dimensions

$$u(z)\,\frac{\partial \chi}{\partial x} = \frac{\partial}{\partial z}\left[K(z)\,\frac{\partial \chi}{\partial z}\right] \qquad (2.19)$$

with the mean wind u(z) blowing along the x-axis. Gifford (1959) has shown that concentration at a point is affected only by sources in a narrow upwind sector of approximately $20^{o}$ and thus justifies the neglect of the cross-wind component in Equation (2.19) and also in Equation (2.18). In order to solve Equation (2.19) analytically,

another physical assumption regarding the restriction of the vertical mixing was made. Whereas in Lettau's model a restrictive layer of air is assumed to be always present over the urban area causing an accumulation of pollutants, in the ATDL model such a restrictive layer is assumed to be high enough to have no effect on the surface concentration in the area. The height of the mixing layer at any distance downwind is assumed to be

$$h^*(x) = 3\,\sigma_z(x) = 3\,ax^b \qquad (2.20)$$

where parameters a and b are functions of atmospheric stability.

The differing assumptions made in the two models are expressed graphically in Figure 2.1. In the concept of a box model the restrictive layer is situated at a constant height $h^*(x)$ over a city causing uniform vertical distribution of pollutants $\chi(z)$ below. However, in the ATDL model it is assumed that the height at which the restrictive layer $h^*(x)$ is situated, grows steadily with the vertical spread of the urban plume downwind. The vertical distribution of pollutants $\chi(z)$ is Gaussian.

If the urban area is divided into a regular pattern of grid squares of unit size $\Delta x$ with N grid squares in the direction of the mean wind, then the concentration in the centre of grid block 0 is the summation over all grid squares upwind of the receptor square and may be expressed as

$$\chi = \frac{z_1^m}{c_1\, u_1\, B\,(1-s)} \left(\frac{\Delta x}{2}\right)^{1-s} \left\{ q_o + \sum_{i=1}^{N} q_i \left[ (2i+1)^{1-s} - (2i-1)^{1-s} \right] \right\} \qquad (2.21)$$

The source streugth in the receptor square is $q_o$ and the source strength in the i-th grid square upwind is $q_i$. Within each grid square the source strength is assumed to be constant. Equation (2.21) has been derived for changing wind speed and eddy diffusivity with height following the simple power laws

$$u(z) = u_1 \left(\frac{z}{z_1}\right)^m \qquad (2.22)$$

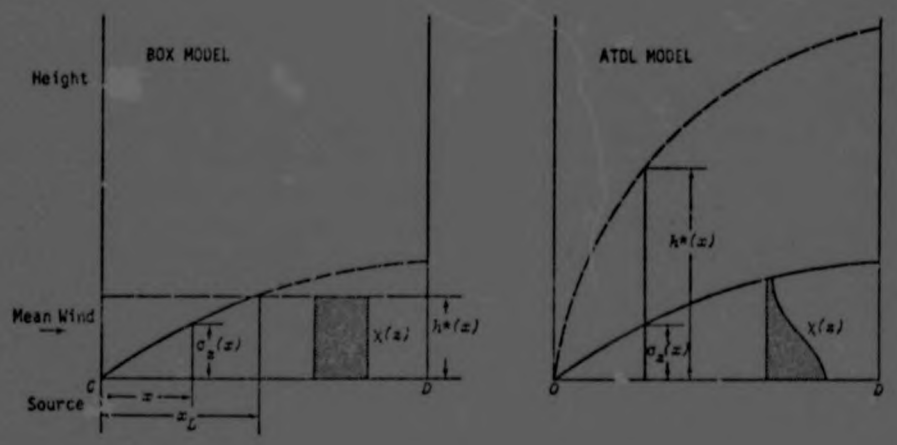



Figure 2.1 Simulated effect of a restrictive elevated layer on the concentration distribution in the box and ATDL models

and

$$K(z) = K_1\left(\frac{z}{z_1}\right)^n \tag{2.23}$$

Parameters m and n are determined experimentally and depend on the stability of the atmosphere, on the surface roughness and also on the choice of the reference height $z_1$. Further, parameters s and $c_1$ in Equation (2.21) may be defined as

$$s = \frac{m + 1}{2 + m - n} \tag{2.24}$$

and

$$c_1 = 3\ a^{\,1/(m+1)} \tag{2.25}$$

The value of parameter B depends on the form of the vertical concentration distribution.

It is a simplified version of the ATDL model that finds most frequent application. The first physical assumption made in the simplification of Equation (2.21) is the assumption of a wind speed u constant with height. The parameter m in Equation (2.22) becomes zero and it may further be shown that, for the condition stated in Equation (2.20), parameter s = b. If vertical concentration distribution of Gaussian form is assumed, the parameter B reads

$$B = \frac{1}{3}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \tag{2.26}$$

and Equation (2.21) becomes

$$\chi = \frac{1}{u\ a\ (1 - b)}\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\left(\frac{\Delta x}{2}\right)^{1-b}\left\{q_o + \sum_{i=1}^{N} q_i\left[(2i + 1)^{1-b} - (2i - 1)^{1-b}\right]\right\} \tag{2.27}$$

For area sources of constant emission strength $q_i = q_o$ Equation

(2.27) reduces to

$$\chi = \frac{q_o}{u\ a\ (1 - b)} \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left[(2N + 1)\left(\frac{\Delta x}{2}\right)\right]^{1-b} \qquad (2.28)$$

and for a given stability and grid size

$$\chi = C \frac{q_o}{u} \qquad (2.29)$$

where

$$C = \frac{1}{a\ (1 - b)} \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left[(2N + 1)\left(\frac{\Delta x}{2}\right)\right]^{1-b} \qquad (2.30)$$

The parameter C is a function of the atmospheric stability and city size. The dependence of C on city size is rather weak, since the exponent (1-b) in the last term of Equation (2.30) is smaller than 0,3 for any stability conditions.

When the parameter C is calculated for various combinations of stability parameters a,b and city diameters D, values close to 50, 200 and 600 are obtained for unstable, neutral and stable conditions and the city size of 10 kilometres. However, when observations in 44 North American cities have been used to determine the annual value of C, an average of 50 has been found to correlate best with the observed levels of atmospheric sulphur dioxide (Gifford and Hanna, 1973).

## 2.3 Similarity theory

The similarity theory originated from the work of Obukhov (1941) and was further developed by Batchelor (1950, 1964), Monin (1959), Gifford (1962) and others. The starting point of the theory is the hypothesis that the Lagrangian (i.e. particles-attached) characteristics of the flow in the surface stress layer depend on the same flow parameters that describe the Eulerian (i.e. relative to a fixed co-ordinate system) characteristics. The parameters are the friction velocity $u_*$ for neutral flow and the Monin-Obukhov length L for flow under diabatic conditions. Dimensional analysis is the basic technique used. It follows from it that the mean vertical displacement $\bar{Z}$ is given by

$$\frac{\overline{dZ}}{dt} = b\, u_* \, \phi\left(\frac{\bar{Z}}{L}\right) \tag{2.31}$$

where b is a universal constant and $\phi$ is a universal function. Correspondingly, the horizontal displacement $\bar{X}$ is given by

$$\frac{\overline{dX}}{dt} = \bar{u}\,(c\bar{Z}) \tag{2.32}$$

where $\bar{u}\,(c\bar{Z})$ is the mean wind speed at the height $(c\bar{Z})$ and c is a universal constant.

In order to determine $\bar{X}$ and $\bar{Z}$ the constants b,c and the $\phi$ function must be specified (Pasquill, 1974). Then the mean concentration distribution of particles is calculated using values of $\bar{X}$ and $\bar{Z}$. For a receptor point located at (x, y, z) and an instantaneous point source of the strength Q, the relationship is given by Gifford (1975) as

$$\bar{\chi}\ (x, y, z, t) = \frac{Q}{(\bar{Z})^3}\ f\left(\frac{x - \bar{X}}{\bar{Z}}\ ,\ \frac{y}{\bar{Z}}\ ,\frac{z - \bar{Z}}{\bar{Z}}\ ,\ \frac{\bar{Z}}{L}\right) \tag{2.33}$$

Equation (2.33) is valid in the surface stress layer. Attempts to extend the validity of the theory above the surface stress layer by considering additional flow parameters such as the geostrophic wind and Coriolis deflection result in greatly increasing the complexity of the dimensional analysis. An application of the similarity theory to estimates of pollutant dispersion in urban areas has been reported by Friedlander and Seinfeld (1969).

## 2.4 Statistical theory

The statistical theory follows the mathematical analysis of properties of a continuously varying entity first suggested by Taylor (1921). When applied to particle velocity components u', v', w', the displacement of a particle after travel time T may be written as

$$\int_0^T dX(t) = \int_0^T v'(t)\, dt \tag{2.34}$$

$$\int_0^T dY(t) = \int_0^T v'(t)\, dt \tag{2.35}$$

$$\int_0^T dZ(t) = \int_0^T w'(t)\, dt \tag{2.36}$$

For the special case of homogeneous and stationary turbulence, i.e. if $\overline{u'^2}$, $\overline{v'^2}$, $\overline{w'^2}$ are constant in space and time and representative of the total turbulent field, the variances of the displacement of a particle at time t are expressed as

$$\overline{X^2}\,(T) = 2\overline{u'^2} \int_0^T \int_0^t R_x\,(\xi)\, d\xi\, dt \tag{2.37}$$

$$\overline{Y^2}\,(T) = 2\overline{v'^2} \int_0^T \int_0^t R_y\,(\xi)\, d\xi\, dt \tag{2.38}$$

$$\overline{Z^2}\,(T) = 2\overline{w'^2} \int_0^T \int_0^t R_z\,(\xi)\, d\xi\, dt \tag{2.39}$$

where $R\,(\xi)$ is the Lagrangian correlation coefficient between particle velocities at times $T_2$ and $T_1$ and

$$\xi = T_2 - T_1 \tag{2.40}$$

As most of the practical problems of atmospheric diffusion are solved in the Eulerian system of coordinates with the pollutants being transported from a fixed-point source past the fixed-point receptor by the mean wind it is necessary to relate the Lagrangian motion as expressed by Equations (2.34) to (2.40) to the Eulerian system. In the following treatment the proposal of linear proportionality between Lagrangian and Eulerian times $\xi$ and t where

$$\xi = \beta t \tag{2.41}$$

is adopted following Hay and Pasquill (Pasquill, 1974). The ratio between the Lagrangian and Eulerian time scales $\beta$ was measured extensively and is known to vary with the thermal state of the atmosphere (Slade, 1968).

The next assumption in the development of a practical model is considered with the distribution of dispersing pollutants. In the Gaussian models discussed here it is assumed that the shape of the concentration distribution is Gaussian along all three coordinate directions. Then, the Gaussian model for calculating the dispersion of airborne pollutants released from an instantaneous point source can be written as

$$\chi(x,y,z,t) = \frac{Q}{(2\pi)^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} \exp\left\{-\frac{1}{2}\left[\frac{(x-\bar{u}t)^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right]\right\} \quad (2.42)$$

where t is the time during which the puff travelled along the mean wind trajectory with the speed $\bar{u}$. In Equation (2.42) the Lagrangian variances of displacement $\bar{X}^2(T)$, $\bar{Y}^2(T)$, $\bar{Z}^2(T)$ have been replaced by Eulerian variances $\sigma_x^2(x)$, $\sigma_y^2(x)$, $\sigma_z^2(x)$ in accordance with the conversion from a Lagrangian to an Eulerian system.

Assuming the turbulent dispersion in the x- direction as expressed by the variance $\sigma_x^2$ to be very small in respect to the transport by the mean wind, terms containing $\sigma_x^2$ may be neglected and the equation for a continuous point source is obtained by integration with respect to time as

$$\chi(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right] \quad (2.43)$$

The variances $\sigma_y^2(x)$ and $\sigma_z^2(x)$ represent the crosswind and vertical dispersion and are determined experimentally as functions of the distance of the plume from the source. Discrete stability classes are often introduced in the process of determining $\sigma_y(x)$ and $\sigma_z(x)$ in order to approximate the changing capacity of the atmosphere to disperse the pollutants. When the source is elevated above the ground at height H, the reflection of the plume from the ground must be included in the model and Equation (2.43) becomes

$$\chi(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \exp\left\{-\frac{1}{2}\left[\frac{(z-H)^2}{\sigma_z^2} + \frac{(z+H)^2}{\sigma_z^2}\right]\right\} \quad (2.44)$$

The Gaussian model as represented by Equations (2.42) to (2.44) has been utilized in many instances to model pollution from multiple sources. In such applications, large isolated sources, such as power generating plants, are usually considered separately and their effects are added to the concentration fields resulting from the multitude of small sources in an urban area. Typically, the urban area is divided into a number of smaller areas, for each of which a uniform source strength may be defined. The area source is represented by a point or line source of equivalent strength. The solution of the basic equations for a set of measured or predicted parameters is obtained at a great number of receptor points for each of the source areas and the results are finally superimposed, yielding the total concentration of pollutants at each receptor point. All require the use of a computer for a period of time proportional to the degree of detail attempted in the respective models.

### 2.4.1 The Gaussian plume model for multiple sources

The first models using the Gaussian plume approach to simulate pollution distribution from multiple sources have been developed by Frenkiel (1956), Pooler (1961), Clarke (1964), Turner (1964), Koogler *et al.* (1967) and Miller and Holzworth (1967). They differ only in detail, one of the most elaborate being the model by Turner (1964). In this model, the area sources are approximated by finite crosswind line sources passing through the centres of the emission squares. The ground concentration at a receptor point (x,y,0) is calculated using the Gaussian plume formula

$$\chi(x,y,0) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{H^2}{\sigma_z^2}\right)\right] \qquad (2.45)$$

In order to be able to consider a finite crosswind line source while still using the simple equation for a point source (Equation 2.45), Turner assumes the length of the line source to equal one quarter of the square size. The length of the crosswind source is then added to the crosswind diffusion parameter $\sigma_y$ for the point source. The height H at which the pollutants are released is adjusted to 20 m for all sources in order to reduce the number of computations required. The source strength Q is taken as equivalent to the total

emission rate in the square. The wind speed u and wind direction are considered constant over each interval of two hours. To account for diurnal changes, all meteorological and emission input parameters are re-evaluated for each interval of two hours. The standard deviations of concentration distributions in the plume $\sigma_y$, $\sigma_z$ are evaluated for differing stability classes according to the scheme introduced by Pasquill (Gifford, 1968, Turner, 1969).

The model has been applied to estimate $SO_2$ concentration levels in an urban area where measurements from 32 monitoring stations were available. It has been found that the calculated concentrations exceeded observed concentrations. The overestimation is especially marked downwind of strong sources (source strengths differed in each source square), while upwind of strong sources the observed values occasionally exceeded calculated concentrations (Turner, 1964).

The overestimation downwind and the underestimation upwind of major sources in particular is due to the approximation of the area source by a single source placed in the centre of the respective area. Sources situated between the upwind edge and the centre of the square are not considered to contribute to the ground concentrations upwind of the centre, and by the time the pollutants pass the centre their actual contribution will be less than calculated. The general overestimation, except for receptors situated immediately upwind of major sources, may be attributed to the assumption of a unique source height of 20 metres. Pollutants released at higher levels will reach the ground much later than calculated or even pass the urban area further downwind.

A more accurate approximation to the area source has been attempted in the model described by TRW Systems Group (1969) and known as the Air Quality model. The area source is approximated by a point source of equivalent strength at such a distance upwind that the $22{,}5^{\circ}$ wind sector subtends the width of the source area (Figure 2.2).

Equation (2.45) remains the governing equation of the model which has been developed for estimates of mean annual concentration levels. Frequency distributions of major meteorological parameters are required for input that includes a combination of 16 discrete wind directions

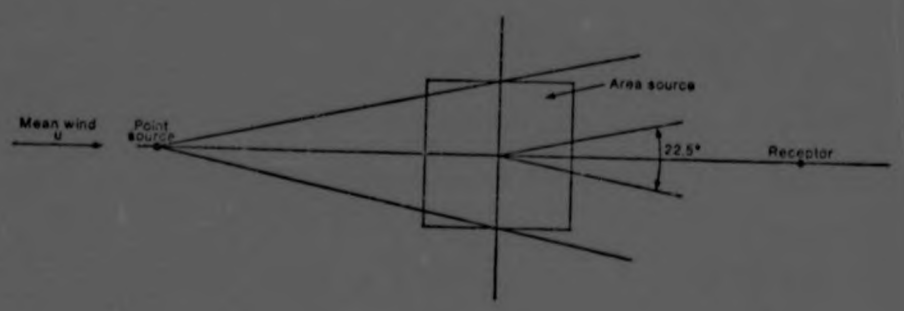



Figure 2.2 Area source approximation by a virtual point source

corresponding to a $22{,}5^{o}$ circular sector, 6 wind speed classes and 5 stability categories. In the Air Quality model the concept of mixing depth is used to consider a possible restriction of vertical spread from large individual sources. The depth of the mixing layer is taken as the annual average of afternoon mixing depths as estimated by Holzworth (1967) and modified for differing stability conditions. For periods when the vertical spread of pollutants is restricted the average ground concentration is calculated as

$$\chi = \frac{Q}{(2\pi)^{\frac{1}{2}} \sigma_y h^* u} \exp\left(-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right) \qquad (2.46)$$

where $h^*$ is depth of the mixing layer through which uniform vertical mixing takes place. The effect of buoyancy on the rise of a hot plume is included for major sources. The height at which pollutants are released from lesser sources is assumed to be uniform and to be equal to the average height of an office or residential building.

The approximation of a multiple (area) source by a point or a line source must be regarded as one of the possible sources of errors especially where the grid squares are large. Fortak (1970) has replaced the area source by a dense and regularly spaced system of point sources and so reduced the grid square size considerably (50 x 50 m). It is obvious that then the approximation of a much smaller area source by a point source will be more representative but it will also increase the computational effort immensely. When a detailed frequency distribution of meteorological parameters, non-constant wind profile and fine temporal resolution are simultaneously included, the computer time required may become prohibitive. The results obtained for Bremen by Fortak (1970) are in a good agreement with observed data but this cannot simply be attributed to the reduced grid size. The city of Bremen is situated in an open and flat terrain with well-definable air movement and therefore more suitable to application of Gaussian plume theory than the majority of other cities.

2.4.2 The Gaussian puff model for multiple sources

If individual releases, so-called puffs, are considered to diffuse separately, the average concentration at a receptor point (x,y,z) is obtained by integration of contributions by all individual puffs. The concentration resulting from one release is given by Roberts et al. (1970) as

$$\chi(x,y,z,t,t') = \frac{Q}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z} \exp -\frac{1}{2}\left\{\frac{[x-\bar{u}(t-t')]^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right\} \tag{2.47}$$

where t' denotes the time of release and t the time at which the concentration is calculated. The variances $\sigma_x^2(t-t'), \sigma_y^2(t-t'), \sigma_z^2(t-t')$ in Equation (2.47) are functions of the travel time (t-t') and must be determined by experiment.

Davidson (1967), Shieh et al. (1970), Roberts et al. (1970), Start and Wendell (1974) have reported the application of the puff concept to studies of urban air pollution levels. The average concentration at receptor point is obtained by integration of contributions from individual puffs over the period of interest. If a puff is released at time t' and position (0,0,0) and $\Delta$ denotes the time interval, then for steady wind in the x-direction the concentration at time $t = m.\Delta$ is given by

$$\chi(x,y,m.\Delta,t') = \sum_{n=1}^{m} Q_{m-n+1} \int_{(n-1).\Delta}^{n.\Delta} \frac{\exp -\frac{1}{2}\left\{\frac{[x-u(t-t')]^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right\}}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z} \tag{2.48}$$

Equation (2.48) can be generalized by introducing the frequency function of f(i,j,k) for variations of wind speed, wind direction and stability.

The critical part of the puff model is the determination of the dispersion coefficients $\sigma_x(t)$, $\sigma_y(t)$, $\sigma_z(t)$. Roberts et al. (1970) assume that $\sigma_x(t) = \sigma_y(t) = \sigma_h(t)$ and derive $\sigma_y(t)$ and $\sigma_z(t)$ from dispersion parameters $\sigma_y(x)$, $\sigma_z(x)$ for plumes where t is the travel time $t = \frac{x}{u}$. Gifford (1968) and Pasquill (1974) have pointed out that the dispersion rate of a small growing puff differs from that of a plume. The plume is regarded as a sum of averaged puffs transported by the mean wind along the x-axis of a fixed co-ordinate system, while the individual puff has its co-ordinate system located along the trajectory and therefore moving all the time. Consequently a distict number and size of eddies will act upon the puff as it travels. At first only few eddies of comparable size to the size of the puff contribute to the spread, whereas the whole spectrum of turbulence diffuses the plume. Later the action of larger and larger eddies on the growing puff increases the dispersion rate to a higher value. Thus the use of $\sigma_y(t)$ and $\sigma_z(t)$ derived from experiments with plumes may bring a substantial error into the calculation. Islitzer and Slade (1968) and more recently Pasquill (1974) summarize the results of experiments with instantaneous releases. The data are still incomplete mainly owing to the practical difficulties associated with simultaneous measurements of instantaneous concentration at a large number of receptors.

The fact that the puff equation (Equation 2.47) does not become infinite but assumes an $x^{-2}$ concentration distribution in calm conditions is often seen as a possible basis for simulation of the dispersion of pollutants under nearly stagnant conditions which cannot be provided by the plume model. However, it should be pointed out that the specification of the dispersion coefficient $\sigma_x$ in the direction of the mean wind is required in order to solve Equation (2.47). In calm conditions the transport by the mean wind ceases to dominate the process and the specification of $\sigma_x$ becomes increasingly important.

## 2.5 Gradient transport theory

The gradient transport theory of turbulent dispersion was initially proposed in analogy with the mixing-length theory of molecular diffusion (Sutton, 1953). The turbulent flow is considered to consist of eddies

which carry mass, momentum and heat and behave like true molecules. Diffusion at a point is related to the gradient of concentration at the same point by assuming that the particle (molecule) is transported down the gradient of concentration at a rate that is proportional to the magnitude of the gradient. This assumption is expressed as

$$F = -K\left(\frac{\partial \bar{\chi}}{\partial n}\right) \tag{2.49}$$

where F is the rate of transport across the surface, K is the coefficient of proportionality and $(\partial\bar{\chi}/\partial n)$ is the gradient. It can be shown (Donaldson, 1973) that for the conditions of parallel shear flow the Equation (2.49) represents a first-order closure model of the second-order terms in Equations (2.1 - 2.4). In the application to the atmosphere, the diffusion equation may be written (Sutton, 1953, Pasquill, 1974) as

$$\frac{d\chi(x,y,z,t)}{dt} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \chi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \chi}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \chi}{\partial z}\right) + Q - R \tag{2.50}$$

where Q represents all sources of a specific pollutant and R is the sum of all processes active in removing the pollutant from the atmosphere. If a number of chemically active pollutants are to be modelled simultaneously, Equation (2.50) may be developed for each pollutant species individually expressing the rate of chemical production or reduction in the last two terms on the right-hand side.

By using Equation (2.50) the effect of turbulent action of the atmosphere on the concentration levels has been reduced to determining the spatial components of the eddy diffusivity K. Analytical expressions for $K_x$, $K_y$, $K_z$ are only available for the shallow surface layer from applications of the similarity theory. As the surface layer represents only a small portion of the polluted atmospheric layer, the eddy diffusivities $K_x$, $K_y$, $K_z$ must be determined experimentally or by using alternative approaches. A general analytical solution of Equation (2.50) for arbitrary forms of the eddy diffusivity and wind profile is not available. Equation (2.50) has been solved analytically for greatly simplified forms of eddy diffusivity and wind profile (for a summary see Appendix A). In order to obtain general solutions of Equations (2.50) numerical techniques must be applied.

2.5.1 Analytical models

The most convenient way to obtain an analytical solution of Equation (2.50) is to assume isotropic diffusion and to disregard spatial variations of eddy diffusivities by writing

$$K_x = K_y = K_z = K = \text{constant} \tag{2.51}$$

The solution of the resulting Fickian equation

$$\frac{d\chi}{dt} = K(\nabla^2\chi) \tag{2.52}$$

for an instantaneous point source of emission strength Q is of Gaussian form (Roberts, 1923)

$$\chi\,(x,y,z,t) = \frac{Q}{(4\pi Kt)^{\frac{3}{2}}} \exp\left[-\frac{(x^2 + y^2 + z^2)}{4\,Kt}\right] \tag{2.53}$$

Solutions for other source configurations may be obtained by integration of Equation (2.53) with respect to time and space.

Most of the experimental data have been obtained for the vertical eddy diffisivity $K_z$ and its variation with height. The experimental evidence of variations of the vertical eddy diffusivity and the wind profile with height has led to further attempts to solve Equation (2.50) analytically. For this purpose Equation (2.50) has been reduced to its two-dimensional form

$$\bar{u}(z)\left(\frac{\partial\chi}{\partial x}\right) = \frac{\partial}{\partial z}\,K_z\left(\frac{\partial\chi}{\partial z}\right) \tag{2.54}$$

The physical assumptions preceding the reduction are those of steady state conditions $\left(\frac{\partial\chi}{\partial t}\right) = 0$, the neglect of diffusion in the x-direction in favour of transport by the mean wind along the x-axis and the removal of the y-component in the presence of an infinite line source. Equation (2.54) has been solved for variations of eddy diffusivity and wind profile, following the simple power law (Equations 2.22 and 2.23). Following Sutton (1953) the solution may be written as

$$\chi\,(x,z) = \frac{Q}{\bar{u}_1\,\Gamma(s)}\left[\frac{\bar{u}_1}{(m-n+2)^2\,K_1\,x}\right]^s \exp\left[-\frac{\bar{u}_1\,z^{m-n+2}}{(m-n+2)^2\,K_1\,x}\right] \tag{2.55}$$

In general little use has been made of analytical solutions of the diffusion equation for the urban air pollution problem. This may mainly be attributed to the difficulties in deriving simple forms for K(z) and u(z) that would be representative for a large urban area, but still simple enough to allow an analytical solution of Equation (2.54).

### 2.5.2 Numerical models

The development of numerical techniques has made the solution of the diffusion equation (Equation 2.50) possible for arbitrary forms of the eddy diffusivity and wind profile and provides a basis for the inclusion of kinetic chemical reactions that are typical for the Los Angeles type of photochemical pollution. Both Eulerian and Lagrangian co-ordinate systems have been utilized in the numerical models.

In the Eulerian model an imaginary, three-dimensional grid system is used to divide the urban area into blocks or cells. Equation (2.50) isdivided into discrete intervals and solved numerically. The concentration in each cell is calculated as the sum of pollutants transported into it from the neighbouring cells by the advective wind and by diffusion and of pollutants released in the cell during the same period of time. The distribution of concentration in the cell is assumed to be uniform. The amount of pollutants that leave the cell for other cells is determined by the wind components at the boundaries and by the gradient of average concentration between the two cells.

The process of dividing the diffusion equation into discrete intervals may be illustrated using the scheme in Figure 2.3. For a uniform size of the grid volume $\Delta V = \Delta x \cdot \Delta y \cdot \Delta z$, the diffusion equation is approximated for the central grid square (i,j,k) by a

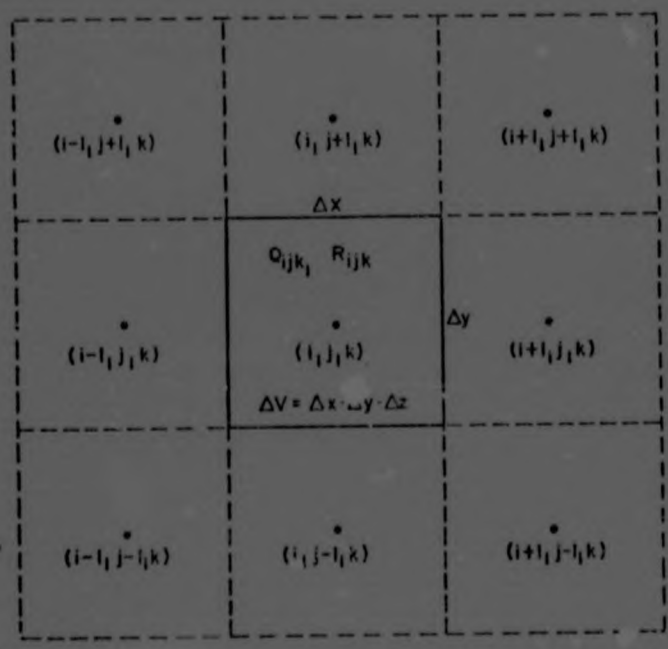



Figure 2.3 A section of the grid system used for dividing the diffusion equation in the numerical model. The x-coordinate of the grid system is parallel to the direction of the advective wind. The source strength and the removal rate in the central volume $\Delta V$ are represented by $Q_{ijk}$ and $R_{ijk}$ respectively

second-order, central finite - difference scheme where the concentration after the (n+1) time step is expressed following Shir and Shieh (1974) as

$$\chi_{ijk}^{n+1} = \chi_{ijk}^{n} + \underbrace{F_x(\chi_{ijk}^{n}) + F_y(\chi_{ijk}) + F_z(\chi_{ijk})}_{a} + \underbrace{D_{xy}(\chi_{ijk}^{n}) + D_z(\chi_{ijk})}_{b} + \underbrace{\frac{\Delta t \cdot Q_{ijk}}{\Delta V}}_{c} - \underbrace{\Delta t \cdot R(\chi_{ijk}^{n})}_{d} \qquad (2.56)$$

The terms a and b on the right-hand side represent the advection and the diffusion process respectively with a source term c and a removal term d completing the equation.

The size of the grid volume is of necessity determined by the available computer capacity and running costs, which will limit the maximum number of grid steps in standard applications. Consequently, a compromise must be reached between the requirements of accuracy and the time of computation, resulting in typical horizontal dimensions of an individual cell of several kilometres. Early finite - difference schemes suffered from the effect of producing artificial diffusion in the advective terms which became significant when the scheme was applied to relatively large grid sizes (Randerson, 1970). A simple demonstration of how the artificial diffusion terms develop illustrates the problem.

If Equation (2.56) is re-written for the x-direction only, it becomes

$$\chi_i^{n+1} = \chi_i^{n} + F_x(\chi_i^{n}) + D_{xy}(\chi_i^{n}) + \frac{\Delta t \cdot Q}{\Delta x} - \Delta t \cdot R(\chi_i^{n}) \qquad (2.57)$$

where $F_x(\chi_i^{n})$ is the advective term. If only the advective term is retained on the right-hand side and is allowed to assume the simplest form of

$$F_x(\chi_i^{n}) = \frac{\bar{u}}{\Delta x} (\chi_i^{n} - \chi_{i-1}^{n}) \Delta t \qquad (2.58)$$

Equation (2.57) bec s

$$\frac{\chi_i^{n+1} - \chi_i^n}{\Delta t} + \frac{\bar{u}}{\Delta x} (\chi_i^n - \chi_{i-1}^n) = 0 \qquad (2.59)$$

where $\Delta x$ is the grid length in the x-direction and $\chi_{i-1}^n$ denotes the concentration in the upwind square at a time interval n. Applying the Taylor's theorem (Pektorys, 1969)

$$f(x_o + h, y_o + k) = f(x_o, y_o) + \frac{(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}) f x_o, y_o}{1!} + \ldots + \frac{(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y})^n f x_o, y_o}{n!} + R_{n+1} \qquad (2.60)$$

to $\chi_i^{n+1}$ and $\chi_{i-1}^n$ and rearranging, Equation (2.59) bc omes

$$\frac{\partial \chi_i^n}{\partial t} + \bar{u} \frac{\partial \chi_i^n}{\partial x} = \bar{u}\left(\frac{\Delta x}{2} - \frac{\bar{u}\Delta t}{2}\right) \frac{\partial^2 \chi_i^n}{\partial x^2} + a_2 \frac{\partial^3 \chi_i^n}{\partial x^3} + \text{higher-order terms} \qquad (2.61)$$

The first term on the right-hand side of Equation (2.61) will increase with increasing grid size $\Delta x$ for given wind speed $\bar{u}$ and time interval $\Delta t$, resulting in a pseudo-diffusion effect caused by introducing the discrete int is. Many alternative schemes such as the higher-order finite-difference schemes and the introduction of finite-element schemes have been developed to minimize the error. The main domain of application of the majority of numerical models has been the modelling of automobile emissions and reactive pollutants in the atmosphere (Mahoney and Egan, 1970, Sklarew et al., 1971, Reynolds et al.,1973, 1974, Pandolfo and Jacobs, 1973, Roth et al., 1974, Shir and Shieh,1974, Ragland and Pierce, 1975, Bankoff and Hanzevack, 1975, MacCracken and Sauter, 1975).

In the Lagrangian (trajectory) model (Eschenroeder and Martinez, 1973, Wayne et al., 1973) an air parcel of constant volume and shape is followed by attaching the co-ordinate system to the parcel as it moves along the trajectory of the advective wi The governing equation of the trajectory model may be obtained by introducing the following transformation of variables into Equation (2.50):

$$\xi = \xi\ (x,y,t)$$
$$\eta = \eta\ (x,y,t)$$
$$z = z \qquad (2.61)$$
$$t = t$$

where $\xi\ (x,y,t)$ and $\eta\ (x,y,t)$ are determined from the constructed trajectories of the advective wind. The resulting equation is again solved numerically. As the air parcel is moving along the trajectory of the wind no flux of pollutants takes place through the parcel's vertical boundary either by advection or by diffusion. Allowance is made for intake of pollutants through the horizontal boundary as the parcel passes over a pollutant source. Mixing and chemical reactions take place inside the parcel. Though this treatment evades the occurence of artificial diffusion terms, the applicability of the Lagrangian model is severely restricted by the initial assumption of a vertical air parcel of constant volume and shape. Thus, the variations of wind speed and direction which commonly occur in urban areas are not considered in the treatment and represent an error source of considerable magnitude. The construction of the trajectories from ground-based data presents an additional problem in this type of model which has found fewer applications than the Eulerian model.

Apart from the numerical problems and the associated extensive computer running times, the main sources of uncertainties in applications of numerical K-theory models are the determination of realistic eddy diffusivity coefficients under a variety of atmospheric conditions and, to a lesser degree, the availability and representativeness of suitable wind flow data for the region of interest.

## 2.6 Discussion

In regression models no attempt is made to solve the problem of turbulent transfer in the atmosphere and hence the process of dispersion of pollutants in an urban area. Instead of physical and mathematical formulation of underlying physical processes, a set of data observed at a specific locality are analysed by statistical means. In the proportional model only variations of the emission rates are considered

Variations of all other parameters describing the state of the atmosphere, the height of release,etc. are not included. The number of variables which enter the equation in empirical models is generally higher, including variations of meteorological parameters, persistence of concentration levels,etc. However, all source data (emission rates, height of release) and their variations are disregarded. The regression models are only applicable to the locality at which the relationship among the variables has been observed. Extensions to other parts of the urban area or even to other areas are not possible. The models give a quick qualitative answer to problems where the possible effect of a change in a major variable such as the emission rate is the main consideration. In research applications they can be used to test the development of a more complex model.

The simple deterministic models are based on a physical approach to the urban diffusion problem. However, the complexity of the models is greatly reduced by the introduction of simplifying assumptions. In the box model a homogeneous source strength is assumed over the entire urban area. The height at which the pollutant is actually released does not enter the calculation and all the emissions are assumed to take place at the ground level. A mean wind speed and wind direction are defined over the whole area and the vertical mixing of pollutants is restricted by the constant presence of a stable layer overhead. As a result a uniform vertical concentration distribution is assumed. The input parameters include the emission rate, the wind speed, the depth of the mixing layer and the size of the urban area. The application of the box model is straightforward with very little computational effort being needed. The model may best be applied to estimates of short-term concentrations in large areas with reasonably uniform emissions and not many major sources at considerable heights above the ground level.

The ATDL model makes use of a grid system to provide a basis for spatial variation of emission rates and the resulting concentrations. Meteorological conditions are not specified for each square separately but are assumed to be uniform over the entire area. The major input parameters include the emissions, the wind speed and wind direction and the atmospheric stability. Large individual sources are treated by the Gaussian plume formula and their contribution to the ground concentration in the centre of each square is added to the contribution by area

sources. The time scales to which the ATDL model may be applied depend on the time interval over which the variations of the atmospheric stability, the wind speed and the emissions remain small. Hence, for typical diurnal changes predictions of short-term concentrations of the order of several hours and very long-term concentrations (seasonal or annual) are adequate. If significant diurnal changes of atmospheric conditions or emission rates must be expected, averaging times of the order of a day will be difficult to apply.

The simple diffusion models are models with limited use in practical applications especially for design and planning schemes and for short-term operational control. They are best suitable for describing the overall effect of an area with small variations in the emission rate on the concentration levels downwind. In research applications the simple models can be used for testing the development of a more complex model.

In the statistical theory of turbulence it is assumed that for a homogeneous flow the distribution of diffusing pollutants is Gaussian. Many methods of dispersion estimates based on the Gaussian distribution have been developed for large elevated sources and later also applied to urban emissions at or near the ground. Large individual sources situated in the urban area are treated separately and the large number of small sources near the ground are lumped into area sources on a grid pattern. Gaussian models differ in the manner in which this source area is represented for dispersion calculation, in the size of the grid and in the detail of input data. Spatial and temporal variations of more input parameters can be considered than in the previous models.

The Gaussian plume model includes several assumptions. First, it is valid for steady-state conditions only. In reality these are never met and are usually approximated by dividing the period of interest into shorter intervals over which the variations of meteorological parameters and emission rates are considered to be small. The averaging times are of the order of several hours or longer, while plume description represents conditions averaged over a time interval of several minutes. Secondly, the effect of wind shear on horizontal diffusion is not considered in the treatment of Gaussian plumes. The neglect of wind shear is small over short distances from the source, but becomes signi-

ficant at greater distances typical for large urban areas. The assumption of constant wind speed over the entire urban area of several tens of kilometres is not adequate, since the trajectories of plumes are much more complex. Thirdly, under nearly stagnant conditions associated with intensive atmospheric stability and low wind speeds, the dispersion of pollutants becomes irregular. The transport by the mean wind ceases to dominate the process and Equation (2.44) becomes infinite as the wind speed approaches zero.Fourthly, the standard deviations of concentration distribution in the Gaussian plume have been obtained from measurements over flat terrain. The values of $\sigma_y$ and $\sigma_z$ are not expected to be representative for plumes travelling over complex topography. Furthermore, the complex topography has a strong effect on the wind structure and often makes the concept of the mean wind unrealistic. Further assumptions made in the Gaussian plume model regard the chemical nature of pollutants. The pollutants are considered to be chemically stable or only slightly reactive, e.g. sulphur dioxide.

The Gaussian puff model provides a basis for a detailed spatial and temporal resolution of wind data by using the method of following the wind trajectory instead of defining mean wind over the entire area. However the wind data available on the average for an urban area are often incomplete. If a very detailed information on the wind structure is used in the model, the same degree of accuracy should be applied to the other input data at the same time. The lack of detailed input information in large urban areas and uncertainties associated with the assessment of the input, particularly the emission estimates on the one hand and the need and cost of extensive computer use on the other, make the application of the Gaussian puff model less practical for urban air pollution problems that the application of the Gaussian plume model.

The application of similarity theory is restricted to the surface layer in which the variation of the shearing stress with height remains small. The depth of the surface stress layer reaches several tens of metres covering only a shallow portion of the total polluted atmospheric layer over an urban area. Attempts to extend the similarity theory above the surface stress layer by considering additional flow parameters greatly increase the complexity of the model.

In the gradient transport theory the transport of pollutants is

assumed to follow the gradient of concentration of the entity at a rate that is proportional to the magnitude of the gradient. The complete solution of the diffusion equation requires specification of the wind profile and eddy diffusivity coefficients. The diffusion equation may be solved analytically for simple forms of u(z) and K(z) only while the horizontal components of turbulence are neglected. In the case of isotropic diffusion and constant eddy diffusivity with height, the solution of the diffusion equation leads to a Gaussian concentration distribution with the variances $\sigma^2 = 2Kt$. As the assumption of constant eddy diffusivity is not met in the atmosphere, variations of eddy diffusivity and wind speed with height have been introduced following the simple power law. The parameters for the power law are determined experimentally. However, the simple power law does not adequately represent the true atmosphere. As complex variations of K(z) and u(z) cannot be incorporated into an analytical solution, numerical methods have to be applied to solve the diffusion equation. Two concepts of coordinate systems are used in numerical models. In the Eulerian approach the concentration equation is divided into discrete intervals and solved numerically in each cell of the three-dimensional grid. In the process a truncation error often occurs in the simulation producing artificial diffusion in the advective term. When the number of grid cells is substantially increased in order to minimize the truncation error extensive computer times are required for the execution of the model. In the Lagrangian approach an air parcel of constant volume and shape is followed as it moves along the trajectory of the advective wind. This treatment evades the production of artificial diffusion during the simulation, but the applicability of the Lagrangian model is restricted by the initial assumption of a vertical air parcel of constant volume and shape to simulations involving constant wind profiles. The practical problem does not rest in excessive computer times, but in the difficulties of constructing adequate wind trajectories from predominantly ground-based experimental data. The main domain of numerical models of gradient transport theory is the simulation of the behaviour of chemically reactive pollutants in city atmospheres.

Attempts have been made to solve the Boussinesq equations for the atmosphere which represent an open system with more unknowns than equations. To close the system higher-order terms are modelled empirically. In spite of a considerable theoretical development several conceptual

and numerical problems still remain to be solved before the model can routinely be applied to simulations of atmospheric pollution in a complex urban area. In addition to conceptual and numerical difficulties, the technique places extensive requirements on the computer size, speed and execution times.

The present state of knowledge concerning the turbulent processes in the atmosphere is reflected in physical aspects of urban air pollution dispersion models. A variety of models have been developed for a variety of applications and in all models idealized conditions are assumed. In contrast to the treatment of isolated elevated sources in which the Gaussian plume model has widely been accepted as the best applicable scheme available, no such a clear distinction exists among the urban models. This necessitates a careful selection of the appropriate modelling technique in each individual application. The nature and density of low-level sources of air pollution and the effect of the city on the dispersive capacity of the atmosphere make the selection of a realistic model difficult. The theoretical difficulties are compounded by the computational effort involved in the simulation and by the multitude of required input data. In order to obtain sufficient boundary conditions for the execution of the models a parameterization of the polluted atmospheric layer is introduced.

# CHAPTER 3

## CHARACTERIZATION OF MODEL PARAMETERS

In the previous chapter the theoretical framework for the modelling of pollutant dispersal processes has been outlined and existing modelling techniques have been reviewed. A variety of model parameters are used together with the mathematical formulation in the dispersion model to specify the boundary conditions in the application to a specific urban area. The main model parameters can be recognized as

- an inventory of pollutant emissions,
- meteorological data,
- geographical parameters, and
- data on atmospheric chemistry of the pollutant species.

### 3.1 Emission inventories

The fact that the concentration of a pollutant may, in the first instance, be linearly equated to the rate at which the pollutant is released, makes the emission inventory a necessary prerequisite to any dispersion modelling effort. An estimate of the amount and distribution of pollutant emissions as well as an estimate of their spatial and temporal variations form the basis of the emission inventory. Given the necessary instrumentation and expertise, either a direct or an indirect method may be used. In the direct method the emission levels are measured *in situ* using stack monitoring devices. This method gives accurate information on each emission source examined, but requires a considerable employment of man-power and instrumentation. The indirect method is based upon estimates from a characteristic information such as the consumption figures and conversion factors for combustion processes, a detailed knowledge of an industrial process or traffic patterns for transportation related problems.

The proportionality between emission rates and concentration levels is closely approximated in a pollution study of a single,

non-reactive or a chemically reactive pollutant such as the particulate matter or sulphur dioxide. However, the linear relationship will dramatically change for reactive pollutants, the best known example being the formation of photochemical smog. Hence the emission estimates for chemically reactive pollutants must also include the information on its chemical predecessors and the reaction rates.

## 3.2 Meteorological parameters

The contribution of an urban source to the concentration of an inert pollutant at a space and time point is determined by the transport and dispersion of the pollutant cloud between this point and the point of release. Thus, a realistic assessment of the parameters which reflect the transport and dispersive properties of the planetary boundary layer over the period of interest is the most important part of a dispersion model. All meteorological parameters are strongly influenced by the time-dependent thermal stratification of the planetary boundary layer.

### 3.2.1 Atmospheric stability

The degree of thermal stratification in the planetary boundary layer has a controlling effect on the capacity of the layer to disperse airborne pollutants. Diabatic processes in the atmosphere give rise to positive or negative buoyancy forces which in turn enhance or damp turbulent motions. The conditions of the boundary layer under which positive buoyancy forces act on the parcel of air as it rises vertically are referred to as unstable. Negative buoyancy forces imply stable conditions. Neutral conditions refer to a layer in which the processes are adiabatic and the buoyancy forces are in a neutral equilibrium. In addition to thermal stratification the degree of atmospheric stability depends on shear effects.

Several theoretical descriptions have been advanced to parameterize the effect of atmospheric stability. The best known parameters are the Richardson number Ri and the Monin-Obukhov length L. Following Sutton (1953), the Richardson number is defined as

$$Ri = \frac{g}{T} \frac{\frac{\partial \theta}{\partial z}}{\left(\frac{\partial u}{\partial z}\right)^2} \qquad (3.1)$$

and indicates the ratio between the rate at which turbulent energy is consumed by buoyant forces and the rate at which turbulent energy is produced by vertical wind shear. In the buoyant term, $\left(\frac{\partial \theta}{\partial z}\right)$ represents the vertical gradient of potential temperature $\theta$, T is the mean absolute temperature of the air and g is the gravitational constant. Vertical wind shear in Equation (3.1) is expressed by the term $(\partial u/\partial z)$. According to the definition of the Richardson number, a turbulent motion will remain turbulent if the rate of production of turbulent energy is greater than its consumption by buoyancy, i.e. $Ri < 1$. The motion will subside into a laminar motion when the ratio is reversed ($Ri > 1$) and more turbulent energy is consumed than produced. The transition between the two regimes should take place when an equivalence between production and consumption ($Ri = 1$) is reached. However, the experimental evidence available (Pasquill, 1974) suggests a wider range of the value at which turbulence is suppressed ($Ri = 0{,}4\text{-}1{,}0$) and a much lower value ($Ri < 0{,}25$) for the initiation of turbulence in the original laminar motion.

The Monin-Obukhov length L is defined (Monin and Obukhov, 1954) as

$$L = - \frac{u_*^3 c_p \rho T}{kgH_f} \qquad (3.2)$$

and expresses the relationship among the buoyancy parameter (g/T), the momentum flux represented by the friction velocity $u_*$ and the heat flux term $(H_f/c_p\rho)$. For upward heat flux ($H_f > 0$) found under unstable conditions the length L is negative. Positive length L indicates a downward heat flux associated with stable conditions and for the heat flux approaching zero the length L becomes infinite.

Although the Richardson number can be measured more easily than the Monin-Obukhov length, it is often advantageous to describe the turbulent state of the atmosphere in terms of the latter. The reason is that the Monin-Obukhov length remains constant with

height above the ground, whereas the Richardson number is variable. The magnitude of the Monin-Obukhov length may be inferred from the measured Richardson number following Golder (1972) as

$$\frac{1}{L} = \frac{Ri}{z} \frac{1}{\phi_m} \qquad (3.3)$$

where $\phi_m$ is a universal function (Appendix B).

Apart from the theoretical expressions the state of a thermally stratified atmosphere has been described in a number of schemes for practical purposes. Pasquill (1961) has classified atmospheric conditions into six discrete stability classes using observations of surface wind velocity, daytime insolation and night-time cloud cover (Table 3.1). In the scheme developed by Singer and Smith (1966) the stability classes have been related to measurements of horizontal wind fluctuations. An excellent review of the main atmospheric stability typing schemes with particular reference to the parameterization of pollutant dispersion has been given by Gifford (1976).

### 3.2.2 Mixing height and temperature profiles

During favourable dispersion conditions the pollutants are carried vertically by turbulent eddies and convection. The depth of the layer in which the vertical mixing is uninhibited is often called the mixing height (Duckworth and Sandberg, 1954, De Marais, 1961a, Holzworth, 1967). The top of the mixing layer is defined as the height at which the vertical fluxes become very small and virtually no pollutants are mixed into the overlying strata (Slade, 1968). The magnitude of the mixing height experiences large diurnal and seasonal variations which are closely related to the daily and seasonal progression of stability regimes. A direct determination of the mixing height may be accomplished by measuring the vertical component of turbulence throughout the layer. In many air pollution studies, however, the mixing height is inferred from measurements of the vertical temperature structure.

Table 3.1. Pasquill scheme for classification of atmospheric stability

| Stability conditions | Pasquill stability categories |
|---|---|
| Extremely unstable | A |
| Moderately unstable | B |
| Slightly unstable | C |
| Neutral | D |
| Slightly stable | E |
| Moderately stable | F |

Key to stability categories

| Surface wind speed (at 10m) ($m\ sec^{-1}$) | Day | | | Night | |
|---|---|---|---|---|---|
| | Incoming solar radiation | | | Thinly overcast or ≥ 4/8 low cloud | ≤ 3/8 cloud |
| | Strong | Moderate | Slight | | |
| < 2 | A | A-B | B | | |
| 2-3 | A-B | B | C | E | F |
| 3-5 | B | B-C | C | D | E |
| 5-6 | C | C-D | D | D | D |
| > 6 | C | D | D | D | D |

The neutral class, D, should be assumed for overcast conditions during day or night.

In the absence of stratification, the temperature decreases with increasing height throughout the planetary boundary layer at the dry-adiabatic lapse rate of $1^{o}C$ per 100 metres. A sharper decrease in the temperature than the dry-adiabatic rate results in the activation of positive buoyancy forces and the reinforcement of vertical motions. Similarly, negative buoyancy forces are activated and the vertical motions are impeded when the decrease is less than the dry-adiabatic lapse rate. Atmospheric strata characterized by a subadiabatic lapse rate are termed inversions (Sutton, 1953).

The knowledge of temperature lapse rates may be used to determine the approximate extent of vertical mixing. In the presence of an elevated stable layer such as a synoptically-induced subsidence inversion the boundary to vertical mixing is set by the base of the inversion. The base and the intensity of an elevated inversion may be determined by examining temperature profiles obtained from standard radiosonde soundings (Holzworth, 1967, Preston-Whyte et al., 1977). Measurements of higher resolution in the first few hundreds of metres above the surface may be obtained from soundings using a tethered balloon system (Slade, 1968). When no elevated inversion is present to impose an obvious restriction on the extent of vertical mixing, alternative methods have to be adopted. Holzworth (1957) has estimated the mixing height as the height at which the measured temperature profile is intersected by the adiabatic extension of the surface temperature. When an inversion occurs in the atmospheric layer adjacent to the surface the vertical mixing of pollutant released into the inversion is inhibited. The occurence of surface-based inversions is particularly high at night during periods of radiative cooling of the surface under low wind conditions. The depth and strength of the inversion may be determined from standard radiosonde soundings (Holzworth, 1967, Tyson et al., 1976) or tethered balloon measurements (Langenberg, 1976).

Often continuous information on the formation and development of inversion structures is needed for short-time dispersion estimates of the order of one hour. A typical example is the development of fumigation conditions following the gradual dissipation of a surface-based inversion in mid-morning (Hewson, 1945, Tyson, 1969). Acoustic sounding of the atmosphere is a remote control technique which has successfully been used for this purpose (McAllister, 1968, Beran et al 1971, Tyson and von Gogh, 1976, von Gogh and Zib, 1978, Tyson et al., 1980). The technique is based upon the capacity of the atmosphere to reflect sound pulse. The reflection of the sound is effected by temperature inhomogeneities associated with variations in the temperature profile (Tatarskii, 1961).

The extent to which the mixing height determined exclusively from the considerations of vertical temperature structure reflects the true mixing conditions is limited. In addition to the variation

of temperature with height, the production of turbulent energy by wind shear significantly contributes to the total dispersive capacity of the atmosphere. In order to include the effect of the wind on the determination of the mixing height and to retain a relative simplicity of the scheme, Smith and Hunt (1978) have estimated the mixing height from the observations of surface wind and cloud amount in addition to the temperature profiles.

### 3.2.3 Dispersion parameters

The process of dispersion by the turbulent action of the atmosphere is parameterized in air pollution models by the introduction of empirically-based dispersion parameters. The dispersion parameters are determined experimentally taking into account the influence of the thermal structure of the atmospheric layer, the wind vector, the distance from the source and the type of terrain over which the experiment has been carried out. Two groups of dispersion parameters have been established over the years in compliance with the requirements of the two most frequently applied dispersion models - the Gaussian and the K-models. In the following discussion, dispersion parameters pertaining to the Gaussian model are denoted by the symbol $\sigma$ and the symbol K is reserved for reference to the gradient transport model.

#### $\sigma$-values

An experimental determination of standard deviations $\sigma_z$ and $\sigma_y$ of the vertical and lateral distribution of pollutant concentration would prove too costly and impractical in all but a few applications. Therefore, several schemes have been proposed to link the available information on atmospheric dispersion to more easily obtainable measurements such as wind characteristics, radiation intensity and cloud cover (Pasquill, 1961, Gifford, 1961, Turner, 1964, Smith, 1968, Klug, 1969, Carpenter et al., 1971, Briggs, 1974). In all the schemes the state of the planetary boundary layer is expressed, with respect to its dispersion potential, in terms of stability categories and related to measurements of the standard deviations. The scheme

originally developed by Pasquill is based on measurements of concentration distribution in plumes released near the surface. Sets of curves representing standard deviations $\sigma_z$ and $\sigma_y$ of vertical and lateral spreading for six Pasquill stability categories and a downwind distance x from the source are shown in Figure 3.1. A similar scheme using measurements of plume dispersion from a tall stack and a different classification of atmospheric stability classes has been proposed (Figure 3.2) by Singer and Smith (1966) and Smith (1968).

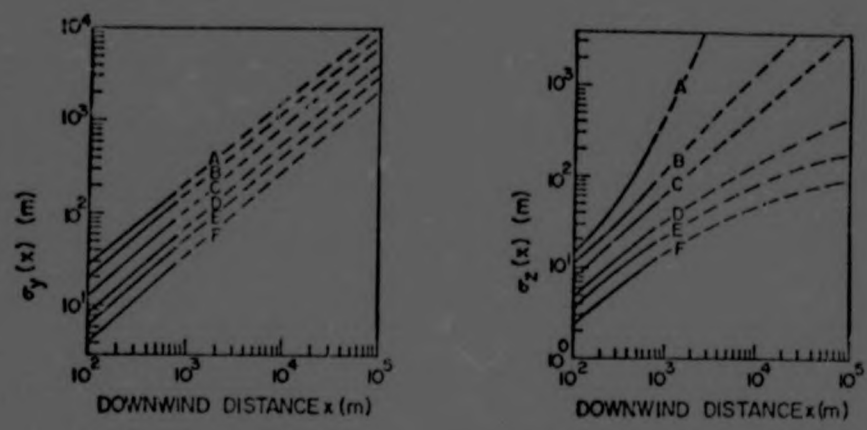



Figure 3.1 Dispersion parameters $\sigma_y(x)$ and $\sigma_z(x)$ as a function of downwind distance x and Pasquill stability categories A - F

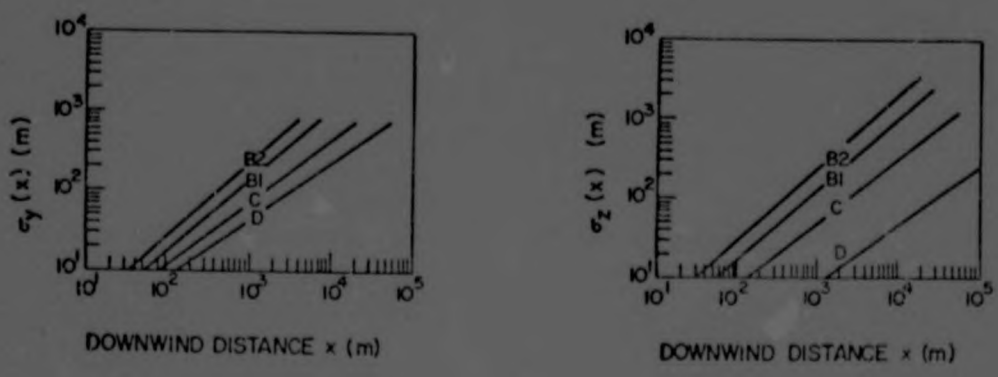



Figure 3.2 Dispersion parameters $\sigma_y(x)$ and $\sigma_z(x)$ for tall stacks as a function of downwind distance x and Singer and Smith stability categories B1 - D

As the original schemes described above are based on measurements obtained in predominantly rural areas, several modifications have been suggested to extend their validity to urban areas. Smith (1972) has modified the original set of Pasquill curves using a surface roughness parameter $z_o$ = 100 cm to simulate the surface conditions in urban areas. The set of modified $\sigma_z$-curves is shown in Figure 3.3. Direct observations of the dispersion process over urban areas have been reported by McElroy and Pooler (1968). Briggs (1974) has made an attempt to reconcile original and recent dispersion experiments in a series of formulae for both rural and urban applications and a wide range of downwind distances. The formulae are tabulated in Table 3.2 and sets of resulting curves are shown in Figure 3.4.

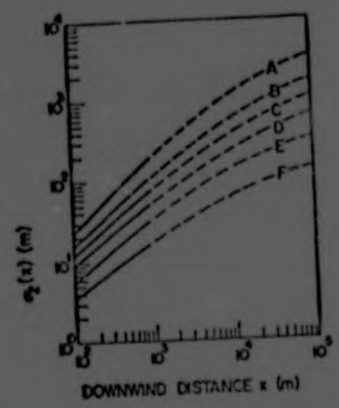



Figure 3.3 Dispersion parameters $\sigma_z(x)$ modified for areas with surface roughness $z_o$ = 1 metre and Pasquill stability categories A - F (after Smith, 1972)

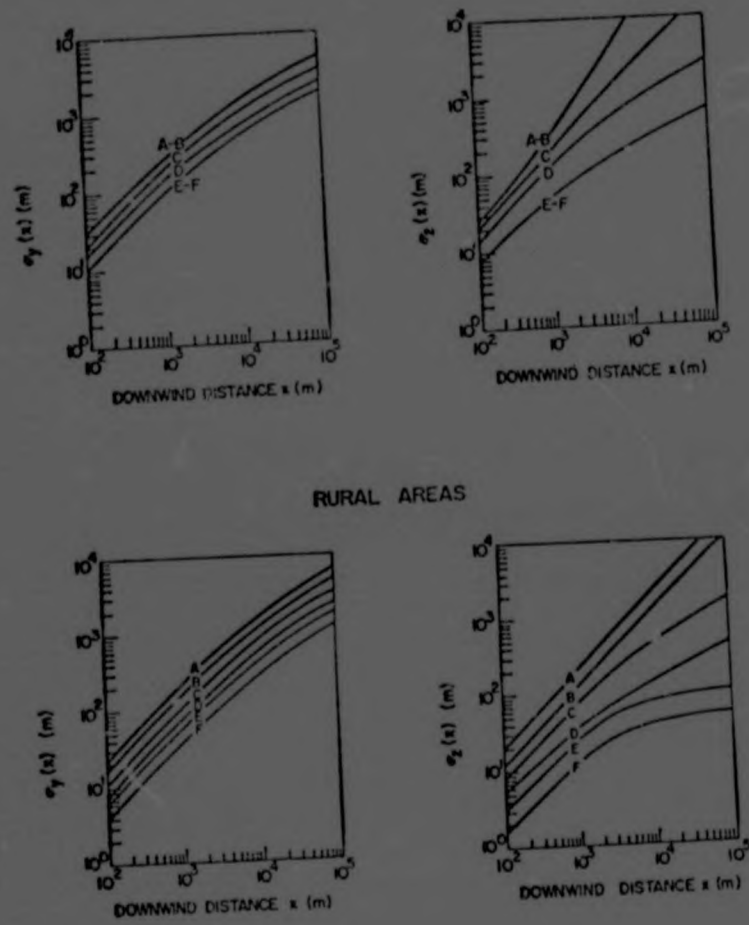



Figure 3.4 Dispersion parameters $\sigma_y(x)$ and $\sigma_z(x)$ based upon the interpolation formulae by Briggs (1974)

K-values

The values of the eddy diffusivity K for use in the gradient transport models also have to be determined experimentally. Several analytical expressions have been proposed to relate the vertical component $K_z$ of the eddy diffusivity to measurements of the wind velocity gradient which can more easily be obtained in the planetary boundary layer. The functional forms of the wind velocity gradient

Table 3.2. Interpolation formulae for determining the disperion parameters $\sigma_y(x)$ and $\sigma_z(x)$ in rural and urban areas (after Briggs, 1974)

| Pasquill category | $\sigma_y$ (x) (metres) | $\sigma_z$ (x) (metres) |
|---|---|---|
| | Rural areas | |
| A | $0.22x(1 + 0.0001x)^{-\frac{1}{2}}$ | $0.20x$ |
| B | $0.16x(1 + 0.0001x)^{-\frac{1}{2}}$ | $0.12x$ |
| C | $0.11x(1 + 0.0001x)^{-\frac{1}{2}}$ | $0.08x(1 + 0.0002x)^{-\frac{1}{2}}$ |
| D | $0.08x(1 + 0.0001x)^{-\frac{1}{2}}$ | $0.06x(1 + 0.0015x)^{-\frac{1}{2}}$ |
| E | $0.06x(1 + 0.0001x)^{-\frac{1}{2}}$ | $0.03x(1 + 0.0003x)^{-1}$ |
| F | $0.04x(1 + 0.0001x)^{-\frac{1}{2}}$ | $0.016x(1 + 0.0003x)^{-1}$ |
| | Urban areas | |
| A-B | $0.32x(1 + 0.0004x)^{-\frac{1}{2}}$ | $0.24x(1 + 0.001x)^{\frac{1}{2}}$ |
| C | $0.22x(1 + 0.0004x)^{-\frac{1}{2}}$ | $0.20x$ |
| D | $0.16x(1 + 0.0004x)^{-\frac{1}{2}}$ | $0.14x(1 + 0.0003x)^{-\frac{1}{2}}$ |
| E-F | $0.11x(1 + 0.0004x)^{-\frac{1}{2}}$ | $0.08x(1 + 0.0015x)^{-\frac{1}{2}}$ |

and eddy diffusivity profiles used for this purpose are summarized in Appendix B.

Little experimental evidence is available concerning the cross-wind component of eddy diffusivity $K_y$. A sensitivity analysis of implemented numerical models (Liu et al., 1976) has indicated a minimal effect of variations in the magnitude of $K_y$ on the predicted concentration levels. The results appear to justify the current use of a constant dispersion parameter $K_y$. As in the Gaussian models, the contribution of the dispersion term to the overall transport of the pollutant in the x-direction is considered too small in proportion to the action of the mean wind.

### 3.2.4 Transport parameters

The general parameter describing the atmospheric transport of pollutants is the wind vector constructed at each space and time point of interest. Two types of flow-field models are invoked to determine the wind information that is required by a dispersion model.

In prognostic models (Deardorff, 1973, Estoque, 1973) attempts are made to solve all pertinent equations for the planetary boundary layer by numerical techniques. The problems encountered in the process of determining an exact four-dimensional flow-field are numerous and often prohibitive. They include the formulation of suitable assumptions to close the set of equations that describe the behaviour of the planetary boundary layer and the subsequent numerical integration of the equations. A detailed discussion of modelling the behaviour of the planetary boundary layer is outside the scope of this study.

In diagnostic models (Dickerson, 1975) the complete set of equations is replaced by the continuity equation to ensure mass consistency within the modelled area. Local observations of wind data from a network of ground-based stations are employed to construct the wind flow pattern. Normally, measurements of the horizontal component of the wind are obtained at a height of approximately 10 metres above the ground and extrapolated vertically by using theoretically or empirically derived wind profiles. Additional physical considerations may be incorporated in order to increase the generality of a diagnostic model.

The wind speed in the planetary boundary layer shows a general increase with height. The wind profile is compounded by the presence of thermally stratified layers such as inversions and by the changing roughness of the surface. Various analytical expressions have been advanced to describe the variation of wind speed with height. A logarithmic profile is often used for conditions of neutral stability and modified for thermally stratified atmosphere by the addition of a linear term. The functional forms of wind profile are discussed in detail in Appendix B. Most of the expressions are too

complex to be used efficiently in dispersion studies. In order not to increase the complexity of an already complex simulation model, simple approximations based upon empirical results have been introduced instead. Calder (1949) has approximated the wind profile by a power law

$$\bar{u}\ (z) \ = \ u_* q \left(\frac{z}{z_o}\right)^{\beta} \qquad (3.4)$$

where q and β are empirical constants. Instead of relating the wind profile to the friction velocity $u_*$ and the surface roughness $z_o$ it is often more convenient to express the velocity at the height z in terms of the mean velocity $u_1$ available from measurements at a known height $z_1$. Then the power law relationship has the form (Sutton, 1953)

$$\frac{\bar{u}\ (z)}{u_1} \ = \ \left(\frac{z}{z_1}\right)^{m} \qquad (3.5)$$

Table 3.3 shows empirical values of the parameter m obtained by De Marrais (1959) for six Pasquill stability classes.

Table 3.3. Values of the parameter m in the simple power law for wind profile (after De Marrais, 1959)

| Pasquill stability category | m |
|---|---|
| A | 0,1 |
| B | 0,15 |
| C | 0,20 |
| D | 0,25 |
| E | 0,25 |
| F | 0,30 |

Jones et al. (1971) have extended the concept of the simple power law to urban areas. In the first 160 metres above the ground they have found a good agreement with observations for

m = 0,2 for slightly stable conditions,
m = 0,21 for neutral conditions, and
m = 0,35 for slightly unstable conditions

### 3.2.5 Plume rise

The distance at which the pollutant plume reaches the surface and the magnitude of the concentration thus produced depend on a number of variables. Turbulent dispersion and advection by the wind have been considered in previous sections. The height of the source from which the pollutant is emitted is another significant factor in the dispersion estimates. The initial momentum of the ejected effluent causes the plume to rise vertically above the release level. This effect is often magnified by buoyant forces acting on the plume when its temperature exceeds that of the ambient atmosphere. The elevation of the plume centreline above the physical height of the source may be included in air pollution dispersion models by adjusting the source height. The effective source height H is defined as the sum of the physical source height h and the plume rise $\Delta h$

$$H = h + \Delta h \qquad (3.6)$$

The plume rise is determined by the plume characteristics particularly the exit velocity of the effluent and its temperature as well as by the ambient meteorological conditions. When the exit velocity of the effluent is high, the initial rate of rise is also high but the momentum diminishes appreciably with the distance. The buoyant forces, however, act continuously on the hot plume as it is advected and dispersed. Under neutral and unstable conditions there is no limit to the plume rise. Under stable conditions, however, the buoyant forces are counteracted by the stable atmosphere until a state of equilibrium is reached. The height at which the equilibrium is reached gives the final rise of the plume. Equations for estimating the plume rise have been derived by many investigators. The available expressions have been reviewed by Briggs (1969). Most of the plume rise equations are given in the form of a power law in which the exponents have been evaluated experimentally. The variables in the equations generally include the buoyancy term, the wind speed

and the downwind distance. Using Briggs' notation the variation of the plume rise with downwind distance may be expressed as

$$\Delta h\ (x) = C\ F^{a}\ u^{b}\ x^{c} \tag{3.7}$$

The buoyancy term in Equation (3.7) is defined following Briggs (1969) as

$$F = \frac{g\ Q_h}{\pi \rho c_p T} \tag{3.8}$$

where $Q_h$ is the heat emission rate, $c_p$ is the specific heat at constant pressure, $\rho$ is the density and T is the temperature of the ambient atmosphere and g is the gravitational constant. The non-dimensional constant C in Equation (3.7) is determined empirically. The value of C = 1,6 has been found to be in good agreement with the experimental data for a variety of stability conditions. Hence, the most frequently applied form of Equation (3.7) for estimating the rise of a hot plume near the source is (Briggs, 1974)

$$\Delta h\ (x) = 1,6\ F^{1/3}\ u^{-1}\ x^{2/3} \tag{3.9}$$

Carpenter et al. (1971) have determined the value of C in Equation (3.7) for a range of stability conditions in dependence on the potential temperature gradient.

In order to determine the final rise of the plume in stable conditions Briggs (1969) has modified the original equation by introducing a stability parameter

$$s = \left(\frac{g}{\theta}\right)\left(\frac{\partial \theta}{\partial z}\right) \tag{3.10}$$

in which $\theta$ is the potential temperature in the stratified layer. The final rise is then expressed as

$$\Delta h = 2,6\left(\frac{F}{us}\right)^{1/3} \tag{3.11}$$

As mentioned earlier the plume rise in neutral or unstable conditions is not contained by the ambient atmosphere and increases with

downwind distance. The plume is, however, continuously dispersed along its trajectory. This effect is approximated for the purpose of dispersion estimates by terminating the calculation of the rise at a certain distance downwind as determined from considerations of the atmospheric turbulence, the buoyancy term and the height of release.

## 3.3 Geographical parameters

The geographical location and the topography of the region in which the modelled area is situated may introduce a great measure of complexity into local dispersion characteristics and cause significant departures from the concentration fields predicted by standard techniques applicable to simple terrain. General climatological parameters such as the mean duration and intensity of solar radiation, the amount and temporal variations of annual precipitation, the altitude and the mean temperature and humidity not only control the daily and seasonal patterns of emission levels, but, more significantly, the process by which the pollutants are removed from the atmosphere or chemically transformed.

The proximity of large water bodies and prominent topographical features is instrumental in the development of specific air flow patterns such as sea and lake breezes and regional topographically-induced winds (Jackson, 1954, Munn, 1966, Tyson and Preston-Whyte, 1972, Preston-Whyte, 1974). Where the urban area itself is situated in complex terrain local topographically-induced conditions prevail. An example of the local topographically-induced air flow is the development of anabatic (upslope) and katabatic (downslope) winds caused by the radiative heating and cooling cycle on sloping surfaces (Munn, 1966, Tyson, 1968). Other examples include air flows that are channeled through the troughs and openings in the local topography and flow separation effects which occur in the wake of significant terrain features (Munn, 1966). A realistic assessment of all these effects is difficult to achieve. The significant phenomena are therefore considered individually in the process of formulating the windfield model.

Modifications of other model parameters such as the dispersion parameters and the shape of plumes have also been observed in very rough, mountainous terrain (Egan, 1975, Start et al., 1975). The observations have been limited to plumes from single elevated rather than multiple low-level sources.

### 3.4 Removal processes and the transformation of pollutants

The final concentration of a given pollutant species at a point in space and time is influenced by a number of processes other than the transport by advection and the dispersion by turbulence and convection. These processes may be described as processes acting towards a decrease in the actual concentration levels by removing the pollutant species from the dispersing plume or transforming it into a different chemical substance. Alternatively, the concentration of a certain pollutant species may rise due to its formation from other chemical substances present in the atmosphere.

If the pollutant is depleted at the rate $\lambda$, its final concentration after the residence time $\Delta t$ is given by Slade (1968) as

$$\chi\ (x, y, z, t) = \chi_o\ (x, y, z, t)\ e^{-\lambda \Delta t} \qquad (3.12)$$

where $\chi_o$ denotes the concentration estimated in the absence of the removal mechanism. The total removal rate is composed of several individual rates which represent a wide spectrum of depletion processes. Chemically stable pollutants are deposited on the surface in their original form. In addition to deposition, reactive pollutants are undergoing chemical transformation during their residence in the atmosphere. The products of the conversion may either be stable or be subject to further chemical reactions.

The principal processes which control the deposition are precipitation scavenging and dry deposition. In precipitation scavenging the pollutant is removed from the atmosphere by rain or snow as well as by other forms of precipitation. The removal may take place either inside the precipitating cloud or between the cloud base and the surface. The dry deposition is effected by the action of gravity, inertia

and diffusion (Hales, 1975). Most of the information regarding the deposition rates is obtained experimentally.

The rate at which a reactive pollutant undergoes chemical transformation depends on its chemical nature, atmospheric conditions and the presence of certain other chemical substances in the polluted air. According to the manner in which the chemical reaction is initiated two principal categories of reactions may be identified. In thermal reactions the process is activated following an increase in the ambient temperature. An example of the thermal reaction is the oxidation of sulphur dioxide in a hot plume. In photochemical reactions the activating energy is obtained by absorption of light. The conversion of atmospheric oxygen into ozone is an example of the primary photochemically-induced transformation. The primary reaction may be followed by a number of secondary reactions resulting in the formation of many new chemical substances. It is often impossible to account for all possible chemical reactions in a dispersion model. Generalized transformation rates have been published by several investigators (Demerjian et al., 1974, Roth et al., 1974, Eliassen and Saltbones, 1975).

# PART II - MODEL APPLICATION

# CHAPTER 4

## APPLICATION OF URBAN AIR POLLUTION DISPERSION MODELS TO PRETORIA

The use of air pollution dispersion models in a new area of application involves the consideration of such specific aspects as the purpose of the application, the nature of the tracer pollutant, the required resolution of model results, the selection of the mathematical description and the detail of available input data. The purpose of the application to Pretoria is to gain an insight into the methodology of dispersion modelling, to evaluate selected techniques and to identify critical model parameters. Based upon the application further refinement of the models will be undertaken.

The selection of Pretoria as the city whose pollution is to be modelled has been based upon its geographical location, climatic conditions and its record of being a city with a high air pollution potential. Sulphur dioxide has been chosen as the tracer pollutant in the study. The time scale to which the models are to be applied has been dictated by the nature of the problem and by the existing legislation related to air pollution. There is a need to simulate long-term concentration levels over the period of a month to a year and longer.

Three models of pollutant dispersion from multiple sources have been selected for application to 1976 and 1977 data for Pretoria. They are the Gaussian plume model for multiple sources, the ATDL-grid model and the Gifford-Hanna simple model. In selecting these models the emphasis has been placed on the varying degree of model complexity with regard to the treatment of multiple sources, while retaining the Gaussian description.

Of the three models, the Gaussian plume model provides the most detailed description of dispersion from the multiple sources. The production of the ground-level concentration is simulated individually at a large number of receptor points using the method of area sources. A uniform height of release is assigned to each area source and the removal of sulphur dioxide from the polluted atmosphere is also simulated.

In the ATDL-grid model the modelled area is divided into a regular array of receptor squares. A mean concentration is estimated in each square assuming ground-level area sources and no removal of the pollutant.

In the Gifford-Hanna simple model the concentration of pollutants from the multiple sources is estimated in proportion to the ratio of the area source strength in the receptor grid square to the mean wind speed. The constant of proportionality is determined experimentally.

In all three models large elevated sources (sources with emission strength greater than 1 g $sec^{-1}$ and minimum height of 30 metres) are treated separately using the Gaussian plume model for point sources. The contribution from the point sources is added to the concentrations produced by the multiple sources yielding the total concentration value.

## 4.1 The application of the Gaussian plume model for multiple sources

When the long-term distribution of pollutant concentration is to be simulated, the continuous changes of the meteorological and dispersive conditions in the atmosphere may be approximated by dividing the period of interest into shorter intervals over which the temporal variations can be considered to be small. The temporal variability of the characteristic parameters is modelled through a sequence of steady-state conditions. The spatial variations of pollutant concentration are approximated by imposing a dense network of receptor points on the modelled area.

In order to obtain a working dispersion model the Gaussian formula for a continuous plume released from an elevated source (Equation 2.44) is further developed. The concentration at a ground-level receptor ($z = 0$) may be expressed as

$$\chi(x, y, 0, H) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp - \left[ \left( \frac{y^2}{2\sigma_y^2} \right) + \left( \frac{H^2}{2\sigma_z^2} \right) \right] \qquad (4.1)$$

where the symbol H denotes the elevation of the source.

In a multiple source environment a fixed receptor point receives contributions from a large number of sources. Invoking the narrow-plume

hypothesis first introduced by Gifford (1959), only contributions from sources situated immediately in a narrow upwind sector are considered at the receptor point. Under this assumption it is possible to develop a frequency function of occurence for winds blowing towards the receptor from a particular direction and to relate the concentration at the receptor point to this frequency distribution.

### 4.1.1 Point sources

The narrow-plume hypothesis also implies that all pollutants released from the sources within a particular wind sector and carried towards the receptor by the wind only mix vertically with the ambient atmosphere. Hence a horizontally integrated contribution is received at the receptor. The integrated crosswind concentration at a ground-level receptor point is obtained by the integration of Equation (4.1) with respect to y from $-\infty$ to $\infty$ as

$$\chi(x, 0, 0, H) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{Q}{u\sigma_z} \exp -\left(\frac{H^2}{2\sigma_z^2}\right) \qquad (4.2)$$

If a unique, spatially uniform wind direction can be defined for each steady-state interval, the mean concentration is related to the frequency function f of the occurence of a particular wind direction as

$$\bar{\chi} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{f}{\left(\frac{2\pi r}{n}\right)} \frac{Q}{u\sigma_z} \exp\left(-\frac{H^2}{2\sigma_z^2}\right) \qquad (4.3)$$

where r is the distance between the receptor and the source and n is the number of sectors of the width $(2\pi r/n)$. In the derivation of Equations (4.2) and (4.3) the wind velocity u has been assumed to remain constant and spatially uniform. As large variations in the magnitude of the wind velocity are likely to occur, the error of defining a constant speed over the period of interest is minimized by the introduction of wind speed classes. For each class the central wind speed is constant and the frequency of occurence of a particular class is incorporated into the composite frequency function. Similarly, the variations of atmospheric stability conditions are approximated through the introduction of stability classes.

The composite frequency function f(i, j, k) describes the frequency with which the pollutants are transported towards the receptor from the i-th sector with the velocity within the range of the j-th class under vertical dispersion conditions represented by the stability class k. The concentration at the receptor point resulting from the release at one location is obtained by summation of Equation (4.3) over J wind speed classes and K stability classes as

$$\bar{\chi} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{n}{2\pi}\right) \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{Q \cdot f(i, j, k)}{r \cdot u(j) \cdot \sigma_z(r,k)} \exp\left[-\frac{H^2}{2\sigma_z^2(r,k)}\right] \quad (4.4)$$

For M sources the total concentration is expressed as

$$\bar{\chi} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{n}{2\pi}\right) \sum_{m=1}^{M} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{Q_m \cdot f(i_m, j, k)}{r_m \cdot u(j) \cdot \sigma_z(r_m,k)} \exp\left[-\frac{H_m^2}{2\sigma_z^2(r_m, k)}\right] \quad (4.5)$$

where the subscript m refers to individual sources and $i_m$ indicates the wind sector in which the source m is located.

If the pollutants are removed from the atmosphere as they travel between the sources and the receptor, the resulting concentration at the receptor will decrease. The decrease for each source-receptor pair depends on the time $\Delta t$ needed by the pollutant to travel the distance and on the removal rate $\lambda$ assuming the simple exponential relationship

$$\bar{\chi} = \bar{\chi}_o \exp^{-\lambda \Delta t} \quad (4.6)$$

The final concentration at the receptor point is obtained by combining Equations (4.5) and (4.6) as

$$\bar{\chi} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{n}{2\pi}\right) \sum_{m=1}^{M} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{Q_m \cdot f(i_m, j, k)}{r_m \cdot u(j) \cdot \sigma_z(r_m, k)} \exp\left[-\frac{H_m^2}{2\sigma_z^2(r_m, k)}\right] \exp(-\lambda \Delta t) \quad (4.7)$$

The model equation for point sources (Equation 4.7) is addressed to situations in which the pollutants mix freely in the vertical as

they travel from the source towards the receptor. The extent of the vertical dispersion is described by the parameter $\sigma_z$. If, however, the vertical mixing is inhibited by the presence of a stably stratified elevated layer along the pollutants path, the effect of the mixing height on the ground-level concentration must be included in the formulation. A detailed method using two parallel reflecting surfaces representing the ground and the top of the mixing layer respectively, has been described by Fortak (1970). The resulting equation is mathematically complicated even for a single source situation. A simple scheme described by Turner (1969) is used instead, in order to keep the execution time of the model within acceptable limits. Turner's scheme begins with the assumption that the ground-level concentration starts being influenced by a restrictive layer situated at the height h* above the ground when the concentration at the base of the restrictive layer reaches one-tenth of the plume centreline concentration. The vertical distribution of concentration begins to change and is assumed to attain uniformity at twice the downwind distance at which the effect of the finite mixing depth started. In analogy to Equation (4.7) for unrestricted dispersion with Gaussian distribution, the ground concentration under conditions leading to uniform vertical distribution is expressed as

$$\bar{\chi} = \left(\frac{n}{2\pi}\right) \sum_{m=1}^{M} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{Q_m \cdot f(i_m, j, k)}{r_m \cdot u(j) \cdot h^2} \exp(-\lambda \delta t) \qquad (4.8)$$

4.1.2 Area sources

The density and the nature of emissions in certain parts of the urban area make an individual assessment of all sources unpractical and prohibitive in terms of computer time. A method of area sources is introduced instead. The area sources are defined on a horizontal grid system of simple geometry as the total amount of pollutants emitted from that area at a constant height. An expression for calculating the contribution of area sources to the ground-level concentration is derived in a form similar to Equation (4.7) using the scheme in Figure 4.1. The total emission rate $Q(r,\phi)$ from the area element at the point $(r,\phi)$ within the area source of a source strength $q(r,\phi)$ is

$$Q(r,\phi) = q(r,\phi)\, r\, dr\, d\phi \tag{4.9}$$

where (r dr dφ) is the area of the element. The contribution of this area element is expressed by Equation (4.4) in which Q has been substituted by Q (r,φ). If the area source is confined within the i-th wind sector, the contribution from a circular arc element at the distance r from the receptor is obtained by integrating Equation (4.4) over the width of the corresponding wind sector as

$$\bar{X} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{n}{2\pi}\right) \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{f(i,j,k)}{r\, u(j) \sigma_z(r,k)} \exp\left[-\frac{H^2}{2\sigma_z^2(r,k)}\right] \int_{\text{i-th sector}} q_i(r,\phi)\, d\phi\, r\, dr \tag{4.10}$$

The subsequent integration with respect to the radial distance r gives the concentration from an area source within the wind sector as

$$\bar{X} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{n}{2\pi}\right) \int_0^{\infty} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{f(i,j,k)}{ru(j)\, \sigma_z(r,k)} \exp\left[-\frac{H^2}{2\sigma_z^2(r,k)}\right] \int_{\text{i-th sector}} q_i(r,\phi)\, d\phi\, r\, dr \tag{4.11}$$

Finally, the total concentration at the receptor is obtained by summation over I wind sectors and by including the removal term as

$$\bar{X} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \left(\frac{n}{2\pi}\right) \int_0^{\infty} \left[ \sum_{i=1}^{I} \int_{\text{i-th sector}} q_i(r,\phi)\, d\phi \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{f(i,j,k)}{u(j)\, \sigma_z(r,k)} \exp\left[-\frac{H^2}{2\sigma_z^2(r,k)}\right] \cdot \exp(-\lambda \Delta t) \right] dr \tag{4.12}$$

Both integrals in Equation (4.12) are evaluated by numerical integration. The stepwise integration of $\int q_i(r,\phi)\, d\phi$ is carried out for finite increments of $\Delta\phi$ along the circular arc at a given radial distance r within the boundaries of a particular wind sector. The integral with respect to r is evaluated next and the integration is repeated for every increment of radial distance $\Delta\phi$ until the contributions of all non-zero area elements have been included in the calculation. The model has been programmed for the

CDC Cyber 174 computer of the CSIR.

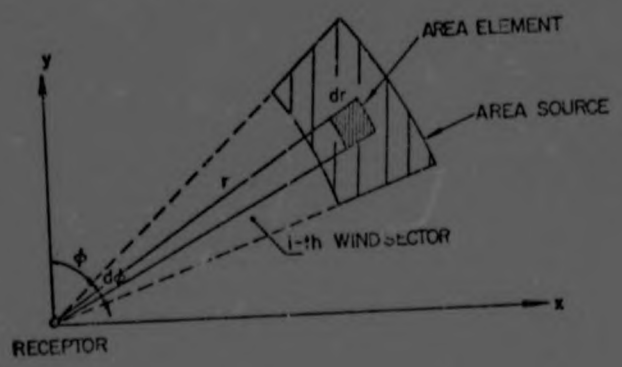



Figure 4.1 The scheme for calculating the contribution of area sources in the Gaussian plume model

### 4.1.3 Input data

#### 4.1.3.1 The geography of Pretoria

Pretoria is situated 25°45' south and 28°12' east on the South African plateau at a mean altitude of 1 400 metres above sea level. The prominent Magaliesberg range in the north and the Langeberg range in the south define a basin in which the main parts of the city are situated (Figure 4.2). Divided by the Daspoort range into two parallel east-west valleys the basin slopes gently towards the north. The major industrial development has taken place to the west of the city centre in the shallower southern valley. Lesser industrial areas are situated in the wider and more clearly defined northern valley. The main suburban development extends over some 15 kilometres east of the commercial and high-density residential centre. Outside the city basin lie scattered residential and light industrial areas while the main ridges remain largely undeveloped. In the extreme east and west are large and densely populated Black residential areas of Mamelodi and Atteridgeville. The total size of the urban area included in this study is 15 kilometres in the north-south and 40 kilometres in the east-west direction.

Situated in the subtropical belt of anticyclonic circulation, the climate of Pretoria is characterized by generally cloudless weather, low relative humidity and high incidence of low wind speeds (Jackson, 1952). This is particularly so in winter when strong radiative cooling of the surface at night results in a high frequency of occurence of temperature inversions in the adjacent atmospheric layer (Tyson et al., 1976). Owing to the sheltered position of Pretoria in the valley, the interaction of synoptic scale circulations with mesoscale winds within the valley system is minimised. In summer, the high pressure cell weakens and the weather becomes more unsettled. The general increase of wind speed is illustrated by July 1977 and January 1978 wind roses for the period from 03h00 to 09h00 in Figure 4.3. Whereas in July light winds from all directions are uniformly represented in the wind rose, a strong easterly component dominates the air flow in January. The increase in the wind activity during the

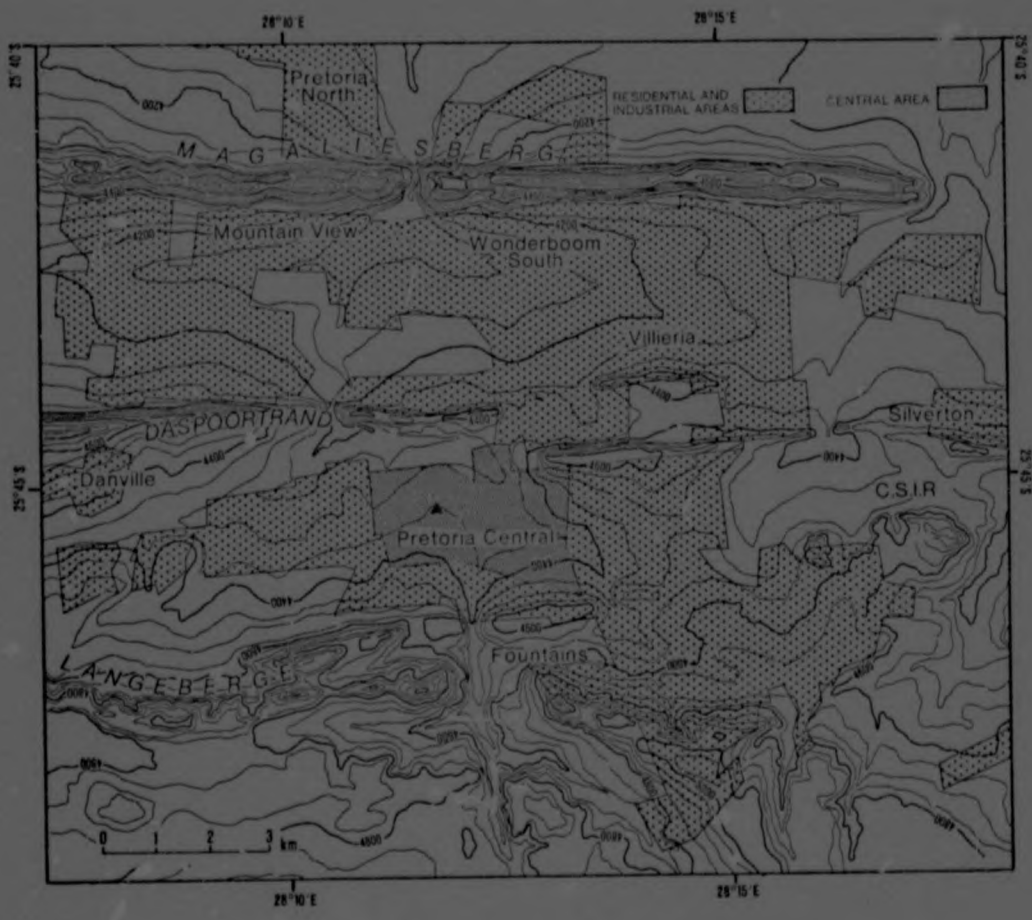



Figure 4.2 The topography and land use of central Pretoria. The contours are in feet (1000 ft = 304,8 m)

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