

TURBULENT PLUME DISPERSAL

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ABSTRACT

A computer method is developed for predicting the dispersal of plumes emanating from point or line sources in a two-dimensional turbulent boundary layer. The method solves the governing partial differential conservation equations by means of a marching finite-difference procedure using a two-grid system to allow for the possibility of widely different scales of the plume and the boundary layer. Closure of the time-averaged, governing transport equations of momentum, thermal energy and concentration of plume material is accomplished via a second-order closure turbulence model which entails solution of further partial differential equations for the turbulent kinetic energy and its dissipation rate together with algebraic relations that permit calculation of the Reynolds stresses and turbulent scalar fluxes.

The turbulence model employed is a variant of an already-existing model. The new developments include modification to account for thermal stratification effects on the turbulence dissipation rate and the turbulent pollutant concentration flux. The transport equation for the latter was also extended to account for situations where a large difference exists between the scales of the concentration fluctuation and those of the fluctuating flow field.

An experimental programme was carried out with the dual purposes of producing experimental data for validating the numerical procedure and to complement existing measurements. The experiments involved measurements of mean con-

centration, mean stream-wise velocity and the Reynolds stresses for a point release in a neutral turbulent boundary layer in a wind tunnel. The effects of a step change in surface roughness downstream of the point of release on the concentration and hydrodynamic fields were examined; also investigated was the effect of height of release on the dispersal over a uniformly-smooth surface.

The numerical procedure was tested by comparing predicted results with corresponding measured ones both in laboratory and atmospheric situations. The predicted results generally displayed good agreement with the experimental data. The only situation where appreciably large disparities occurred between predicted and measured results was in the calculation of the lateral spread of a plume in the atmosphere; in which case the prediction underestimated the observed values. The disagreement was attributed to effects of changes of mean wind direction on a time scale large compared to that of the turbulence which are inherent in the observed data but are not accounted for in the method as it now stands. Suggestions are made for removing this deficiency.

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CHAPTER 1

INTRODUCTION

The history of effluent dispersal studies dates back to the first world war when predictive tools were being applied to assess the dangers that would occur in case of chemical warfare. Ever since that time such studies have been intensified in order to cope with the mounting problem of atmospheric pollution which accompanied expansion of industrialisation and motorisation.

The investigations made on plume dispersal in the atmosphere have included both theoretical and experimental approaches; with the latter serving two purposes; first to obtain empirical formulae that describe the diffusion and secondly to allow assessment of theoretical models. Initially most of the experiments carried out were field studies; although these give valuable information, they are, due to the capricious nature of atmospheric conditions, uncontrollable and are furthermore expensive to perform. These drawbacks tempted experimentalists to attempt to simulate atmospheric diffusion phenomena in wind-tunnels (e.g. Solal (1972), Robins (1975), Poreh (1961)).

With the arrival of digital computers and with the feasibility of employing numerical solution techniques, many of the mathematical difficulties encountered in obtaining analytical solutions to the governing equation of the diffusion process, which had hitherto impeded theoretical approaches were by-passed. With these difficulties removed it has been

possible to incorporate more realistic assumptions into the analysis and this has enabled much better simulation and understanding of dispersal phenomena.

The present study is an extension to the numerical schemes and physical models that had previously been developed at Imperial College. These methods have so far proved successful in several engineering applications (for example Bergeles (1976), Serageldin (1977)) and their employment in environmental studies such as atmospheric plume dispersal, could prove rewarding.

In what follows a brief description of the air flow in the atmospheric layer is given as further background and then a survey is provided of previous studies of plume dispersion in the atmosphere.

1.1 Characteristic features of air motion in the atmosphere

The initiation of large scale motions of air relative to the earth's surface is caused by pressure gradients, that are generated by an uneven distribution of temperature across the surface. Close to the equator intense energy from the sun heats the surface which in turn heats the adjacent air, causing it to rise by the action of buoyancy forces. Near the poles the situation is reversed and instead the overlying air is cooled by the ground and in the process of losing energy causes a descending motion. This state of affairs produces the pressure gradients which cause a movement of air in the general direction of the equator in the lower part of the atmosphere and away from the equator in the upper region.

Once the air is set in motion, the inertial force resulting from the rotation of the earth commences to influence the flow pattern. Further alterations to this large scale motion (known as the 'macroscale') are provoked by major features of the earth's surface such as continents, high mountain ranges, oceans etc., and also by heat and mass transfer occurring over large surface areas.

Macroscale motion can span distances of the order of thousands of kilometers and may persist for days and even months. Superimposed on the large scale motions are smaller scale ones which are induced by local topographical conditions. The smallest of these scales is known as the 'microscale' and ranges in size from millimeters to a few kilometers. It is these scales that will be of most interest in the present study.

From the standpoint of air motion the atmosphere can be separated vertically into two regions: the 'geostrophic layer' and the 'planetary boundary layer', the geostrophic layer lies above a certain height h , defined as the location above which the effect of ground shear stress becomes negligible and is normally in the range of 500 - 1000 m. The magnitude of h is influenced primarily by the thermal stability of the atmosphere and the character of the underlying topography. Lower values of h corresponding to conditions where the ground is aerodynamically 'smooth' and the atmosphere is stably stratified i.e. with the temperature decreasing with height at a rate less than the adiabatic lapse rate.*

*The adiabatic lapse rate is the rate of temperature change with height of a parcel of air which rises or falls adiabatically and has always the same density as its surroundings.

Within the geostrophic layer the dominant forces are the pressure gradient and the force resulting from the Coriolis component of acceleration: these forces, being in equilibrium, result in a motion which is directed along the isobars (i.e. constant pressure lines).

Extending from the ground to the height h is the planetary boundary layer, in which the air is still influenced by the ground friction force and a balance between shear, pressure and Coriolis forces are usually assumed to exist. The influence of the shear force causes the wind direction to veer from its geostrophic state; the angle between the wind direction and the isobars increases as the ground is approached due to the increase of the frictional forces. Over open terrain the angle between wind direction and isobars, near the ground is usually between $10 - 20^\circ$ and can reach higher values if the shear stress increases due to rough topography. The variation of wind direction with altitude is known as the Ekman spiral, and the region over which the direction of the wind changes appreciably is the Ekman layer.

Close to the ground the pressure gradient and Coriolis forces have less influence than the shear stress and are usually neglected (c.f. Lumley and Panofsky (1964)); for non-accelerating flows this gives rise to a constant stress layer which is referred to as the 'surface layer'. From dimensional arguments and consideration of boundary conditions the following logarithmic law can be shown (c.f. Blackadar and Tennekes (1968)) to describe the variation of the mean wind velocity for a neutral flow in the surface layer:

$$\frac{\bar{U}_1}{u_*} = \frac{1}{\kappa} \ln \frac{x_3}{x_0} \quad (1.1)$$

where*: $\bar{U}_1$ is the mean velocity in the direction of x_1 , x_3 is the cartesian coordinate in the vertical direction (with x_1 defined as the direction of the ground shear stress τ and x_2 is the normal to the x_3x_1 plane), x_0 is the effective height of the ground roughness, κ is the Von-Karman constant and u_* is the friction velocity related to τ and the density ρ , by

$$u_* = \sqrt{\tau/\rho} \quad (1.2)$$

Equation (1.1) is identical in form to equations describing the mean velocity in what is termed the 'logarithmic region' of turbulent boundary layers as found by wind-tunnel experiments. In fact in many aspects the wind-tunnel boundary layer does resemble the surface layer. This similarity has led researchers (e.g. Arya and Plate (1971), Schon (1974)) to investigate the modelling of the surface layer by way of wind-tunnel results.

1.2 Review of theoretical studies on diffusion processes

Theoretical analyses of the dispersal of material released into turbulent flows has followed two main lines,

*In general $\bar{U}_i$ will refer to the mean, Eulerian velocity component in the x_i direction while u_i will refer to the fluctuating component. Overbars will henceforth, unless otherwise stated, define ensemble averaged quantities.

usually referred to as: (i) the 'statistical approach' and (ii) the 'transfer theory approach'. In (i) the diffusion is described in terms of the statistical properties of the turbulent motion by following the motion of fluid particles in a Lagrangian fashion. In approach (ii) the partial differential equation describing the conservation of mass of the constituents of the dispersant are solved subject to the appropriate boundary and initial conditions; the equations solved always imply some physical model to represent the transfer of material by turbulent motion.

Further details of these two methods of analysis will now be given.

1.2.1 Statistical approach

G.I. Taylor (1921) was probably the first to express mathematically the migration of particles in a turbulent flow. By analysing the random motion of a fluid particle, in a steady homogeneous turbulent field and considering the ensemble of like particles, Taylor produced his renowned formula for the distance y_i in the i direction travelled by the particles in time t :

$$\overline{y}_{(i)}^2 = 2\overline{v}_{(i)}^2 \int_0^t \int_0^{t'} R_L(\xi) d\xi dt' \quad (1.3)$$

v_i is the Lagrangian fluctuating velocity (for homogeneous turbulence $\overline{v}_{(i)}^2 = \overline{u}_{(i)}^2$) and $R_L(\xi)$ is the Lagrangian auto-correlation coefficient defined as

$$R_L(\xi) = \overline{v_{(i)}(t) v_{(i)}(t+\xi)} / \overline{v_i^2} \quad (1.4)$$

In equations (1.3) and (1.4) the bracketed subscripts indicate that no summation over i is implied.

Equation (1.3) was extended by Batchelor (1949) to three dimensional diffusion for which the generalised dispersion of a particle at time t is represented by the second-order tensor:

$$\overline{y_i y_j} = \int_0^t \int_0^{t'} (S_{ij}(\xi) + S_{ji}(\xi)) d\xi dt' \quad (1.5)$$

where S_{ij} is the correlation

$$S_{ij} = \overline{v_i(t) v_j(t+\xi)} \quad (1.6)$$

Returning to equation (1.3), Taylor (1921) used this to predict the behaviour of $\overline{y_{(i)}^2}$ under the limiting conditions of very small and very large diffusion times. In the former case

$$R_L(\xi) \approx 1$$

and the integral on the right-hand side of equation (1.3) can be carried out to give

$$\overline{y_{(i)}^2} \approx \overline{v_{(i)}^2} t^2 \quad (1.7)$$

with the assumption that the Lagrangian integral time scale

Λ_L , defined as

$$\Lambda_L = \int_0^{\infty} R_L(\xi) d\xi \quad (1.8)$$

is finite, the condition of large diffusion time reduces equation (1.3) to

$$\bar{Y}_{(i)}^2 \approx 2\bar{V}_{(i)}^2 \Lambda_L t \quad (1.9)$$

It is interesting to notice that, in spite of the difference in mechanism between turbulent diffusion and that due to molecular action (in which diffusion is considered to proceed with uncorrelated steps equal to the mean free path) equation (1.9) does resemble that of molecular dispersal, with Λ_L representing the mean free path and $\bar{V}_{(i)}^2$ the square of the molecular velocity.

If as in the kinetic theory of gases, $\bar{Y}_{(i)}^2/2t$ is equated to a diffusivity K_i , then according to equation (1.7) for short diffusion time t , K_i will initially increase linearly with time and according to equation (1.9) it will eventually reach a constant value for long diffusion times. This result will act as a guide in assessing one of the models discussed in the present study.

To describe the variation of $R_L(\xi)$ between the two limiting conditions of large and small diffusion times t , Sutton (1953) assumed that $R_L(\xi)$ primarily depends on $\bar{u}_{(i)}^2$, the kinematic viscosity ν and ξ , and thus obtained from dimensional reasoning:

$$R_L(\xi) = f\left(\frac{v}{\bar{u}_{(i)}^2 \xi}\right) \quad (1.10)$$

f being an undefined function required to satisfy the conditions $R_L(0) = 1$ and $R_L(\infty) = 0$. The form of f given by Sutton to comply with these is:

$$R_L(\xi) = (v/(v + \bar{u}_{(i)}^2 \xi))^n \quad (1.11)$$

where n is a positive integer. If a power law variation of the velocity $\bar{U}_1$ with height is assumed i.e.

$$\frac{\bar{U}_1}{\bar{U}_r} = \left(\frac{x_3}{x_r}\right)^m \quad (1.12)$$

where U_r is a reference velocity at height x_r . Sutton (1953) showed, by employing the mixing length hypothesis (c.f. Sutton (1953), Hinze (1975)) together with equation (1.3), that m is related to n by:

$$m = n/(2 - n) \quad (1.13)$$

If Sutton's (1953) assumptions are correct, one important consequence of equation (1.13) is that the behaviour of $R_L(\xi)$ could be inferred from simple measurements of the velocity profiles in the atmospheric boundary layer.

In a situation where the turbulence is assumed to be independant of molecular effects Sutton (1953) introduced the concept of a microviscosity N , defined as

$$N = u_* x_o \quad (1.14)$$

To replace the molecular viscosity in equation (1.11).

Fundamental criticism (c.f. Slade (1968)) to Sutton's model is that the supposed variation of $\bar{U}_1$ with height contradicts the assumption of homogeneity underlying Taylor's equation (1.3). Moreover, the use of the values of the power index m which makes equation (1.12) approximate the real variation of $\bar{U}_1$ in the atmosphere (i.e. $0 < n < 1$), produces an infinite integral length scale Λ_L . It is further argued in Appendix A1 that the parameters chosen by Sutton to describe $R_L(\xi)$ are inadequate.

In practice, Sutton's model has been widely employed, however Barad and Haugen (1959) deduced from their field experiments that the diffusion pattern cannot be characterised by a single parameter n but rather requires two values for n , one corresponding to the lateral diffusion and the other to the vertical process. Also, their results show that to obtain good agreement with diffusion experiments equation (1.13) should not be used to specify n .

Based on an analysis given by Kamp de Fariet (quoted in Hinze (1975) and Monin and Yaglom (1975)) Hay and Pasquill (1959) presented a method of calculating $\bar{y}_{(i)}^2$ from meteorological recordings of the velocity fluctuations. It was shown by Kamp de Fariet that equation (1.3) can be re-written as :

$$\bar{y}_{(i)}^2 = 2\bar{v}_{(i)}^2 \int_0^t d\xi(t-\xi) \int_0^\infty E_L(n) \cos 2\pi n \xi dn \quad (1.16)$$

where $E_L(n)$ is Lagrangian energy density spectrum of v_i .

Carrying out the outer integration yields:

$$\bar{Y}_{(i)}^2 = \bar{v}_{(i)}^2 t^2 \int_0^{\infty} E_L(n) \left(\frac{\sin(\pi n t)}{\pi n t} \right)^2 dn \quad (1.17)$$

It was then assumed by these workers that the Lagrangian correlation coefficient decays with time in a similar fashion to the decay of Eulerian correlation $R_E(t)$, but with a different time scale, i.e.:

$$R_L(\xi) = R_E(t) \quad (1.18)$$

Here $\xi = Bt$, where B is the ratio of Lagrangian to Eulerian time scales. Equation (1.18) would give the following relation between the Lagrangian energy spectrum $E_L(n)$ and the Eulerian spectrum $E_E(n)$

$$E_L(n) = E_E(Bn) \quad (1.19)$$

Substitution of this result into Equation (1.17) yields

$$\bar{Y}_{(i)}^2 = \bar{v}_{(i)}^2 t^2 \int_0^{\infty} E_E(n) \left(\frac{\sin(\pi n t/B)}{\pi n t/B} \right)^2 dn \quad (1.20)$$

Hay and Pasquill (1959) pointed out that the weighing function $(\sin(\pi n t/B)) / (\pi n t/B)^2$ in Equation (1.20) resembles the effect of averaging the raw data over intervals of time t/B . This result gives a practical means of calculating $\bar{Y}_{(i)}^2$

from measured energy spectrum of v_i .

A study of the contribution of energy at different frequencies to the diffusion process can be made via Equation (1.20) in the two limits when t is very small or very large. In the former case Equation (1.20) gives

$$\bar{y}_{(i)}^2 = \bar{v}_{(i)}^2 t^2 \int_0^{\infty} E_E(n) \, dn \quad (1.21)$$

i.e. all frequencies to the turbulence spectrum contribute to $\bar{y}_{(i)}^2$. In the other limit when t is large it can be shown (c.f. Hinze (1975)) that

$$\bar{y}_{(i)}^2 \approx \bar{v}_{(i)}^2 t E_L(0)/2 \quad (1.22)$$

which indicates that only the small frequency components are contributing to $\bar{y}_{(i)}^2$.

So far the diffusion process discussed has been that of a single particle relative to a fixed co-ordinate frame. Such analyses cannot give any information on the relative position (or relative diffusion) of two or more diffusing particles. Relative diffusion becomes important when, for example, dispersal of a cloud of fluid particles is being studied. Richardson (1926) was the first to introduce the concept of relative diffusion, which Batchelor (1950), later expressed in mathematical terms by examining the separation (in the i direction) vector s_i between two 'tagged' particles moving in a steady homogeneous turbulent field. By forming the ensemble of $s_{(i)}^2$ over an ensemble of like parti-

cles, Batchelor (1950) showed that the rate of increase of $\bar{s}_{(i)}^2$ during the motion at time t is

$$\frac{d}{dt} \bar{s}_{(i)}^2 = 2 \int_0^t \overline{\delta v_{(i)}(t) \delta v_{(i)}(t')} dt' \quad (1.23)$$

where $\delta v_i(t)$ is the relative velocity in the i direction between the two particles.

For conditions when t is small and $\sqrt{\bar{s}_i^2} < l_e$, where l_e is the length scale of eddies in the inertial subrange, Batchelor (1950) argues that since, only eddies having length scales comparable in size to $\sqrt{\bar{s}_i^2}(t)$ contribute to δv_i , then Kolmogoroff's similarity theory of small scale motion (c.f. Batchelor (1959)) can be applied to aid in the description of $\bar{s}_{(i)}^2$. From dimensional reasoning Batchelor then gives

$$\frac{d}{dt} \bar{s}^2 = vG \left(\frac{I \epsilon^{\frac{1}{4}}}{v^{\frac{3}{4}}}, \frac{t \epsilon^{\frac{1}{2}}}{v^{\frac{1}{4}}} \right) \quad (1.24)$$

where ϵ is the dissipation rate of turbulence kinetic energy, I_0 is the initial vector separating the two particles at time $t = 0$ and G is a universal function which is given, for small and intermediate ranges of t , by Batchelor (1949).

In the limit when t is very large and $\sqrt{\bar{s}_i^2}$ becomes larger than Λ_L , Batchelor (1950) argues that the motion of the two particles becomes uncorrelated and ultimately

$$\frac{d}{dt} \bar{s}_{(i)}^2 \rightarrow 2 \frac{d}{dt} \bar{y}_{(i)}^2 \quad (1.25)$$

While the extent of the spread of the plume is assessed through the value of $\bar{y}_{(i)}^2$, it is still necessary to know the distribution of the concentration of pollutant in the plume. Estimation of these distributions from knowledge of $\bar{y}_{(i)}^2$ is normally achieved by speculating on the shape of the probability density distribution of y_i denoted by $P(y_i)$. Batchelor (1949), Frenkiel (1952) and others have assumed that in a steady homogeneous turbulent field $P(y_i)$ follows a Gaussian distribution. In the absence of molecular diffusion the mean concentration resulting from a release from a point source is proportional to the probability density function and hence is also normally distributed. Strictly speaking, $P(y_i)$ has a Gaussian distribution only for short or long diffusion times, in the latter situation the diffusion time must be much larger than the integral time scale Λ_L , and in such a case the statistical central limit theory can be applied (c.f. Lumley (1972), Monin and Yaglom (1977)) to prove the Gaussian distribution assumption. When short diffusion times are considered, the probability density of y_i will be approximately similar to that of u_i (c.f. Monin and Yaglom (1977)) which was shown by Townsend (1947) to be quite close to Gaussian. Although there is no reason to expect that for moderate values of t , $P(y_i)$ would be Gaussian, Townsend's (1951) experiments have shown this to be approximately correct.

For the case of a pollutant being emitted from a continuous point source of strength Q , into a homogeneous turbulent field, the assumption of a Gaussian distribution

yields the following equation for the pollutant concentration $\bar{C}$ (c.f. Fleishman and Frankiel (1955))

$$\bar{C} = \int_{-\infty}^t \frac{Q}{2\pi^{3/2} (\bar{y}_1^2 \bar{y}_2^2 \bar{y}_3^2)^{1/2}} \exp \left[-\frac{1}{2} \left[\frac{(x_1 - \bar{U}_1(t - t_o))^2}{\bar{y}_1^2} + \frac{\bar{x}_2^2}{\bar{y}_2^2} + \frac{\bar{x}_3^2}{\bar{y}_3^2} \right] \right] dt_o \quad (1.26)$$

If diffusion in the mean flow direction is neglected by comparison to transport by mean wind, then equation (1.26) reduces to* (Slade (1968))

$$\bar{C} = \frac{Q}{2\pi \bar{U}_1 \sigma_2 \sigma_3} \exp \left[-\frac{1}{2} \left[\frac{\bar{x}_2^2}{\sigma_2^2} + \frac{\bar{x}_3^2}{\sigma_3^2} \right] \right] \quad (1.27)$$

As can be seen from Equation (1.27) the concentration distribution is completely determined, by specifying σ_2 and σ_3 , once Q and $\bar{U}_1$ are known. The most common approach used in practice to determine σ_2 and σ_3 is from field experiments (c.f. Slade (1968), Pasquill (1974), Smith (1968)) however other methods (e.g. that of Sutton (1953)) are also employed.

Equation (1.27) and the underlying theory are widely referred to as the 'Gaussian plume model' which has been for some time the most popular approach to predicting plume dispersal in the atmosphere. Other forms of Equation (1.27)

*Values of $\sqrt{y_{(i)}^2}$ will henceforth be referred to as σ_i .

that take account of ground effects, elevated sources ... etc. have been proposed; a summary of these can be found in Slade (1968).

1.2.2 Transport Theory

This method of analysis is based on the solution of the ensemble averaged partial differential equation governing the transport of material concentration: it has the advantage over statistical methods that non-homogeneity of both the mean velocity and the turbulence variables can be more easily accounted for.

If the molecular diffusion is neglected the ensemble-averaged partial differential equation representing the conservation of a certain species can be written as*

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial}{\partial x_i} \bar{U}_i \bar{C} = \frac{\partial}{\partial x_i} \overline{u_i c} \quad (1.28)$$

where Einstein summation convention is assumed to hold when repeated indices appear.

The major difficulty in utilising Equation (1.28) to solve the concentration field lies in determining the turbulent fluxes $\overline{u_1 c}$, $\overline{u_2 c}$ etc.: this is sometimes referred to as the 'closure problem'. To this end a 'physical model' (or turbulence model) is employed, which relates the unknown fluxes to quantities which can be

*More details are given in Chapter 2.

obtained. Some of the various models which have been proposed will now be reviewed.

In 1915 Taylor (1915), probably inspired by the kinetic theory of gases, introduced the concept of an 'eddy conductivity'* to play a similar role in turbulent diffusion as that played by the molecular diffusivity in laminar diffusion. According to this concept the turbulent flux $\overline{u_i c}$ can then be written as

$$\overline{u_i c} = - K_{(i)} \frac{\partial \overline{C}}{\partial x_{(i)}} \quad (1.29)$$

where K_i is the eddy conductivity in the x_i direction.

Taylor envisaged that the transfer of a property C by turbulent motion is achieved by the migration of fluid parcels from one layer, 'a' say, in the flow field to another adjacent layer 'b'; for the transfer to occur, Taylor argues, that it is necessary for a gradient of $\overline{C}$ to exist across the two layers. During its motion from a to b the parcel is assumed not to mix with its immediate surroundings i.e. C is conserved and all mixing is achieved at $b^{\pm}$.

With the further assumption that changes in $\overline{C}$ across a distance comparable to the distance from a to b is much

*Boussinesq (1877) had earlier introduced a similar concept for the 'eddy viscosity'.

$\pm$ The mechanism by which the mixing is assumed to occur, was not expounded by Taylor.

smaller than the value of $\bar{C}$, Taylor showed that then K_i can be written as

$$K_i = \frac{1}{2} V_i l_c \quad (1.30)$$

where l_c is the distance from a to b and V_i is a representative velocity of the turbulent flow.

Taylor (1915) did not use Equation (1.30) to calculate K_i but rather matched the solution of Equation (1.28), obtained under certain assumptions, with measurements of C to deduce K_i .

Based on a similar concept to that of Taylor, Prandtl (1925) analysed the transport of momentum with the further assumptions that: (i) the longitudinal and vertical velocity fluctuations are of the same order of magnitude and (ii) the correlation coefficient defined by:

$$R = \frac{\overline{u_1 u_3}}{\sqrt{\overline{u_3^2}} \sqrt{\overline{u_1^2}}} \quad (1.31)$$

satisfy the inequality

$$0 < R < 1$$

Then $\overline{u_1 u_3}$ can be written as

$$\overline{u_1 u_3} = - l_m^2 \frac{\partial \bar{U}_1}{\partial x_3} \left| \frac{\partial U_1}{\partial x_3} \right| \quad (1.32)$$

where l_m has an analogous meaning to l_c and is termed the 'mixing length'. Equation (1.32) implies a velocity scale $l_m \left| \frac{\partial \bar{U}_1}{\partial x_3} \right|$ and a length scale l_m , which give an 'eddy viscosity':

$$\mu_t = \rho l_m^2 \left| \frac{\partial \bar{U}_1}{\partial x_3} \right| \quad (1.33)$$

Prandtl suggested that for flows near solid boundaries l_m should be proportional to the distance, from the point considered, to the nearest surface, and this seems to be borne out by experiments. Since the original formulation of the theory numerous empirical extrusions have been made leading to mixing-length formulae that take account of effects such as compressibility, pressure gradient, laminar/turbulent transition etc. on the behaviour of the wall boundary layer. A useful account of these developments is given by Reynolds and Cebeci (1976).

Once μ_t is known then the eddy diffusivity K_i is normally obtained by assuming it proportional to μ_t/ρ (c.f. Launder and Spalding (1972)) with the coefficient of proportionality equal to Schmidt number* Sc_t i.e.

$$K_i = \mu_t / \rho Sc_t \quad (1.34)$$

Sc_t is obtained by reference to experimental data. A similar definition to Sc_t exists for a turbulent Prandtl number Pr_t when heat transfer is considered thus

$$Pr_t = \mu_t / \rho \Gamma_t \quad (1.35)$$

* K_i as used here is not assumed to depend on direction, the suffix i is left only because of the convention used.

where Γ_t is the turbulent thermal diffusivity.

In spite of its vast use, in both practical application and research work, of the eddy-diffusivity model, it has come under heavy criticism. The fundamental objections can be briefly summarised as follows:

- (i) The assumption that the length scale* of the turbulence (l_c in Equation (1.30)) is much smaller than that of the mean field is seldom valid.
- (ii) During the flight of a fluid parcel the transferable quantity cannot be conserved since mixing can occur by molecular action. Furthermore, sources and sinks of the property in question can exist as for example chemical reaction, when chemically reacting pollutants are considered.
- (iii) Experiments have shown (c.f. Hanjalic and Launder (1972a)) that in some situations a transferable quantity can be transported by turbulence in the absence of a gradient in the mean of that quantity contrary to what was assumed by Taylor.

When the Prandtl mixing length model is employed the following further objections may be raised:

- (iv) According to this model the eddy conductivity will be zero in regions where the velocity gradient (and thus μ_t) is zero. This implication conflicts, in some situations, with experimental observation (c.f. Launder and Spalding (1972)).
- (v) The mixing-length model implies that the production rate of turbulence kinetic energy is proportional to its dissipation rate and that can be expected only when the flow is self-preserving.

Practical problems also arise when employing eddy diffusivity models in that they require considerable empirical input (especially in three dimensional situations) which can only be inferred from measurement in conditions of similar nature to that being predicted.

Despite the criticism however, it must be stated that the eddy diffusivity models have been used over a long period of time and in many instances with considerable success.

To remedy some of the drawbacks of the mixing length model, Prandtl (1945) has proposed, that instead of calculating the turbulent velocity scale V_t by relating it to the mean velocity gradient, V_t should be obtained by solving a transport equation for the turbulence kinetic energy. V_t is then related to k by:

$$V_t = \sqrt{k} \quad (1.36)$$

Hence μ_t can be expressed as

$$\mu_t \propto \rho k^{\frac{1}{2}} l' \quad (1.37)$$

where l' is a length scale of the turbulence and is calculated in a similar fashion to l_m .

The advantage of Prandtl's (1945) proposal, over the mixing length model, is that solution of the equation of k enables account to be taken of the influence of neighbouring regions (by transport effects) on the local value of k .

*This is implied from Taylor's assumption of having small variation of C during the parcel's flight.

Moreover when transport of scalars by turbulent action is considered, the eddy diffusivity is not necessarily zero in regions where the mean velocity vanishes (as would be when the mixing length model is employed). Turbulence models involving the solution of a single equation to characterise the turbulence field are referred to as one equation models.

An immediate extension of Prandtl's one equation model is a two equation model, where a second transport equation is solved for a variable that will either directly or indirectly define the length scale l' . Several variables have been proposed for such a task (for an account of these see Launder and Spalding (1972)). Probably the most employed is the dissipation rate of turbulence kinetic energy ϵ (c.f. Harlow and Nakayama (1968), Jones and Launder (1972)). The attractiveness of solving for ϵ is that it appears directly in the equation of the turbulence kinetic energy and also together with k they define the turbulence length scale viz.

$$l' \propto k^{\frac{3}{2}}/\epsilon \quad (1.38)$$

The use of this two-equation model (sometimes identified as the k - ϵ model) avoids the disadvantages (iv) and (v) mentioned in connection with the mixing length model and also reduces the amount of empiricism required; however because μ_t is completely defined by scalar quantities (k , ρ and ϵ) it is itself a scalar (even in three dimensional flows) and

thus it follows that the eddy conductivity of heat and mass Γ_t and K_i are independent of direction*; this result is contrary to the experimental observations of Quarmby and Quirk (1972). In employing the k- ϵ model to predict scalar transport it is still necessary to obtain the Schmidt or/and Prandtl numbers by appeal to experimental data.

Returning now to the analysis, insertion of Equation (1.29) in (1.28) alters the transport equation of $\bar{C}$ to:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial \bar{U}_i \bar{C}}{\partial x_i} = \frac{\partial}{\partial x_j} K_{(j)} \frac{\partial \bar{C}}{\partial x_j} \quad (1.39)$$

Roberts (1923) gives the solution to Equation (1.39) for a steady point source in a homogeneous turbulent field (which implies a constant K_j) flowing with a constant mean velocity $\bar{U}_1$. If diffusion in the longitudinal direction is neglected and $\sqrt{x_2^2 + x_3^2} \ll x_1$, the result can be written as

$$\bar{C} = \frac{Q \exp \left[-\frac{\bar{U}_1}{4x_1} \left(\frac{x_2^2}{K_2} + \frac{x_3^2}{K_3} \right) \right]}{4\pi (K_2 K_3)^{\frac{1}{2}} x_1} \quad (1.40)$$

If, as mentioned earlier, $\frac{1}{2}\sigma_{(1)}^2/t$ is set equal to K_1 then it is easily verified that Equation (1.40) is identical to (1.27); according to Equation (1.9) at long diffusion times, $\sigma_{(1)}^2$ is proportional to t and therefore K_1 can be assumed constant. However at short times, $\sigma_{(1)}^2$ varies as t^2 and hence K_1 cannot be regarded as constant; this last statement breaks one of the premises on which the solution (1.40)

*Unless Prandtl and Schmidt numbers that depend on direction are defined.

is based.

Other analytical solutions have been obtained to Equation (1.39) under more general assumptions about the velocity and diffusivity distributions. For example Calder (1949) quotes a solution due to Roberts for the case of a continuous line source located at ground level, into a boundary layer in which the velocity $\bar{U}_1$ was assumed to vary according to the following law appropriate to smooth terrain:

$$\frac{\bar{U}_1}{\bar{u}_*} = q (u_* x_3 / \nu)^\alpha \quad (1.41)$$

Here q and α are constants prescribed so as to fit the observed velocity distribution in the region of interest.

For rough surfaces the following formula for $\bar{U}_1$ was adopted

$$\frac{\bar{U}_1}{\bar{u}_*} = q \left(\frac{x_3 - d}{x_o} \right)^\alpha \quad (1.42)$$

where q and α having similar meaning as q and α above, but for a rough wall, d is a constant that depends on the character of the roughness.

The value of K_3 , adopted by Calder, was in all cases assumed equal to the eddy viscosity (i.e. the turbulent Schmidt number was taken as unity) which was obtained from the equation

$$\mu_t = -\tau / \partial \bar{U}_1 / \partial x_3 \quad (1.43)$$

where the shear stress τ was assumed invariant with height.

Davies (1950) obtained the solution to the equation

$$\bar{U}_1 \frac{\partial \bar{C}}{\partial x_1} = \frac{\partial}{\partial x_2} K_2 \frac{\partial \bar{C}}{\partial x_2} + \frac{\partial}{\partial x_3} K_3 \frac{\partial \bar{C}}{\partial x_3} \quad (1.44)$$

for a point source located at ground level under the assumption that $\bar{U}_1$, K_2 and K_3 vary according to the following power laws

$$\frac{\bar{U}_1}{\bar{U}_r} = \left[\frac{x_3}{x_r} \right]^m \quad (1.45)$$

$$K_2 = a_2 \bar{U}_1^{\frac{1-m}{1+m}} x_3^\alpha \quad (1.46)$$

$$K_3 = a_3 \bar{U}_1^{\frac{1-m}{1+m}} x_3^{1-m} \quad (1.47)$$

Here $\bar{U}_r$ is a reference velocity at height x_r , a_3 and m constants which are changed to approximate observed velocity profiles, α is a constant inferred from diffusion experiments and a_2 is a coefficient which depends on α . The analytical solution of Davies is restricted to cases where $\alpha = m$ otherwise a numerical procedure must be used at a certain stage of the analysis.

Analytical methods are not able to cope with the forms of the diffusion equation appropriate to weather conditions encountered in the atmosphere because of mathematical difficulties. This drawback coupled with the advent of large digital computers has led research workers to eschew

analytical methods and instead employ numerical solution procedures, examples of which will now be described.

Ragland and Dennis (1975) obtained numerical solutions to Equation (1.44), by employing a fully implicit finite-difference scheme. In their analysis they specified the velocity and vertical diffusivity as functions which took account of type (stable, unstable or neutral) and degree of stratification, distance from the ground and degree of surface roughness. The lateral diffusivity was assumed proportional to the vertical diffusivity and to the square of the ratio of lateral to the vertical plume spread, i.e.

$$K_2 = K_3 \left[\frac{\sigma_2}{\sigma_3} \right]^2 \quad (1.48)$$

where the ratio σ_2/σ_3 was obtained from field studies given by Turner (1970). Ragland and Dennis (1975) employed their method to predict the dispersal from an elevated point source in a one-dimensional boundary layer (with the velocity varying only in the vertical direction). The results seem to be physically plausible however, no quantitative conclusion can be made because no comparisons with experimental data were given.

Another numerical approach was developed by Pepper and Lee (1970) who used Patankar and Spalding (1967) finite difference procedure to solve simultaneously the transport equations of concentration, temperature, velocity and turbulence kinetic energy. Solution of the latter equation allowed them to calculate the eddy viscosity by assuming that the turbulent shear stress $\overline{u_1 u_3}$ is proportional to

the turbulence kinetic energy k ; thus

$$\overline{u_1 u_3} = -\frac{\mu_t}{\rho} \frac{\partial \bar{U}_1}{\partial x_3} = -0.3k$$

or

$$\mu_t = -0.3k\rho/\partial\bar{U}_1/\partial x_3 \quad (1.49)$$

μ_t was then employed to calculate K_3 and the eddy conductivity of temperature Γ_3 via assumed constant values of the Schmidt and Prandtl numbers respectively (the authors reported that the value of the Prandtl and Schmidt numbers employed was between 0.5 and 1.0. The exact value, however, was not quoted). Pepper and Lee compared their predictions, of a line source in an unstably stratified boundary layer, with the experiments of Malhotra and Cermak* (1964). The results they presented were of concentration profiles at different downstream locations. In general the predicted profiles compared fairly well with the experiments, displaying a maximum deviation of about 20%.

Wassel and Catton (1977) employed a modified version of Patankar and Spalding (1967) two dimensional numerical procedure to predict concentration fields, down-wind of a line source in a two dimensional boundary layer. For their physical model they applied a version of the mixing length

*Malhotra and Cermak's (1964) experiments were basically for a point source, however they proposed a method of numerically integrating the point source data to yield line source plumes.

hypothesis; in which account was taken of thermal stratification. The turbulent diffusivities of heat and concentration were obtained by specifying constant values of the turbulent Prandtl and Schmidt numbers of 0.9. Comparisons made with Poreh and Cermak's⁽¹⁹⁶⁴⁾ experimental results showed an agreement within 15%.

Barnes (1972) employed Patankar and Spalding's (1971) three dimensional, parabolic, numerical procedure which incorporated a $k - \epsilon$ turbulence model. The values of K_2 and K_3 were assumed equal and were obtained from Equation (1.34) by specifying a constant Schmidt number. Barnes (1972) attempted to predict a point source in a two dimensional boundary layer; his results revealed a lateral spread of the plume which was approximately equal to the vertical spread; this is contrary to the experimental observation of Davar (1961), Solal (1972) and others, which generally indicate a larger lateral spread. The disagreement of Barnes' (1972) predictions with experimental findings can be attributed to the isotropic diffusivities employed in the predictions.

Kumar (1978) transferred Equation (1.44) into a set of integral differential equations and solved, employing a marching finite-difference scheme, for the zero, first and second moments of $\bar{C}$ in the x_2 and x_3 directions. The moments in the x_i directions are defined respectively as

$$C_i^0 = \int_{-\infty}^{\infty} \bar{C} dx_i$$

$$C_i^1 = \int_{-\infty}^{\infty} \bar{C}x_{(i)} dx_{(i)}$$

$$C_i^2 = \int_{-\infty}^{\infty} \bar{C}x_{(i)} x_{(i)} dx_i$$

where the superscripts on C refer to the moment and the subscript to the direction of the moment. σ_2 and σ_3 are related to the moments by the following equation

$$\sigma_i = \sqrt{\frac{C_i^2}{C_i^0} - \left(\frac{C_i^1}{C_i^0}\right)^2} \quad (1.50)$$

In the calculation procedure the diffusivities K_2 and K_3 were assumed equal and were specified. Kumar's (1978) predictions of σ_2 and σ_3 revealed large discrepancies (reaching about 250%), from Pasquill's field experiments (c.f. Pasquill (1974)). Some of the discrepancies observed may again be attributed to the isotropic diffusivities employed.

1.3 Present study

1.3.1 Objective

The overall objective of the present investigation is to develop and validate a computer prediction method for the plume dispersal problem under certain specified conditions, described below.

The specific aim is to predict the situation depicted in figure 1.1, which shows a contaminant released from a

point or line source at an arbitrary height into a steady two dimensional turbulent boundary layer which has arbitrary thickness and mainstream velocity. The flow field may be isothermal or thermally stratified in a stable or unstable manner. Variations are allowed in the conditions, in the mainstream direction, such as changes in mainstream velocity and the roughness and heat transfer rates at the surface.

1.3.2 Outline of present contribution

The method of approach is based on the numerical solution of the partial differential equations governing the transport of momentum, thermal energy, contaminant concentration, turbulent kinetic energy and its dissipation rate. The latter two variables were employed together with further algebraic equations, to describe the turbulent transport of the different variables mentioned.

Motivated by a lack of comprehensive experimental data, a brief experimental program has also been undertaken to provide measurements of dispersion from a point source in a neutral turbulent flow over both smooth and non-uniformly rough surface. The following is a brief account of the detailed contributions in the fields mentioned.

(a) Turbulence modelling: The model employed here is basically similar to that suggested by Launder (1975); however some modifications and extensions have been made to the treatment of the turbulent pollutant transport flux to account for thermal stratification effects and situations where large differentials exist between the length scales

of the hydrodynamic and concentration fields further modifications are also proposed to the dissipation rate equation to allow for effects of unstable-stratification.

(b) Numerical methods: A simple marching solution procedure has been developed that is particularly suited for atmospheric diffusion predictions, the main features of which are:

(i) The hydrodynamic and concentration field are solved on separate grids; the two grids can expand or contract so that they just encompass the regions of interest.

(ii) The hydrodynamic and temperature fields are solved as two dimensional variables while the concentration field can be either two or three dimensional.

(c) Experimental study: The measurement programme was aimed at producing experimental data mainly for the purpose of validation of the present numerical procedure and also to complement existing measurements. The quantities measured and conditions comprised:

(i) Concentration measurements downstream of a point source emitted at ground level into a turbulent boundary layer flowing over a smooth surface.

(ii) As in (i) but with a surface which undergoes a step change from smooth to rough.

(iii) Concentration measurements for an elevated release, with the flow being over a continuously-smooth surface.

In all cases hydrodynamic measurements were also made of the mean velocities and the turbulent stresses $\overline{u_1^2}$, $\overline{u_2^2}$, $\overline{u_3^2}$ and $\overline{u_1 u_3}$. In all the cases investigated the streamwise pressure gradient was kept constant and no stratification effects were considered.

1.3.3 Layout of thesis

The remaining part of the thesis contains six further chapters. Chapter 2 deals with the governing equation of mean momentum, mass, thermal energy and concentration; these three equations are presented together with the underlying assumptions. In Chapter 3 the turbulence model employed to calculate the turbulent transport of the above mentioned quantities is derived. Following this, in Chapter 4, the solution procedure for the equation of Chapters 2 and 3 is outlined; also discussed there is the imposition of the boundary conditions and accuracy of the numerical procedure. Chapter 5 is concerned with the description of the experimental programme and the presentation of some of the experimental data obtained, the remainder being presented in Chapter 6, where the experimental and numerically-predicted results are compared and discussed. Finally, Chapter 7 summarises the conclusion of the study and makes recommendations for further work.

CHAPTER 2

THE BASIC EQUATIONS OF AIR MOTION AND POLLUTANT DISPERSAL PROCESSES

In this chapter the differential equations which are assumed to govern the flow in the atmospheric boundary layer and a contaminant therein will be developed.

The governing equations are first presented in their general form in Section 2.1. In the subsequent 3 Sections (2.2 - 2.4) a series of manipulations will be applied to these equations, that will finally reduce them to the versions employed in the present study. In Section 2.2 the equations are transformed into what are termed the 'Boussinesq equations'. These are then averaged in Section 2.3. Finally in Section 2.4 an order of magnitude analysis is carried out on the averaged equations to assess the relative significance of the various terms.

Due to ambiguities associated with application of the averaging process to atmospheric flows, Section 2.5 will be devoted to an examination of this process. It will transpire from Section 2.5 that time averages should be employed; however in the meantime, averages will be assumed to be taken over an ensemble.

In Section 2.7 a summary of the averaged equations in their final form is presented.

2.1 General governing equations of variables considered

The motion of the air in the atmospheric layer can, in dry conditions, be adequately described by the differential conservation equations of momentum, mass and total energy together with the equation of state. These, together with the differential equation expressing the conservation of a pollutant constituent form the basic set in the present study.

The above-mentioned equations will be given here in Cartesian tensor notation, with no distinction made between covariant and contravariant tensors. Figure 2.1 illustrates the frame of reference employed, there the coordinate system $ox_1x_2x_3$ are assumed to be stationary on the earth's surface; with the latter revolving about an 'inertial' axis x'_3 with an angular velocity Ω . As previously defined, the x_1 axis is oriented in the direction of the mean wind at ground level, x_3 is defined as perpendicular to the earth's surface and x_2 is of course normal to the plane x_1x_3 . The equations are then as follows.

Momentum conservation. In the formulation of this equation, the only body forces which are considered are those due to gravity and the artificial forces resulting from the rotation of the frame of reference (see Batchelor (1967)). The momentum equation for a Newtonian fluid, also known as Navier-Stokes equation, can in these circumstances be written as*:

*The compact suffix notation $\phi_{,i} \equiv \partial\phi/\partial x_i$, $\phi_{,t} \equiv \partial\phi/\partial t$ where ϕ is any variable will be employed.

$$\rho U_{i,t} + \rho U_j U_{i,j} = - P_{,i} + [\mu (U_{i,j} + U_{j,i}) - \frac{1}{3} \mu \delta_{ij} U_{k,k}]_{,j} - \rho \Omega^2 \epsilon_{ijk} \epsilon_{klm} e_{sj} e_{tl} e_{nm} \frac{\lambda}{s} \frac{\lambda}{t} z_n - 2\Omega \rho \epsilon_{ijk} e_{sj} \frac{\lambda}{s} U_k - \rho g n_i \quad (2.1)$$

where: P is the pressure, e_{sj} is the cosine of the angle between the stationary $o'x'_s$ axis and the rotating axis ox_j , z_n is the position vector of the fluid element considered relative to O' , g is the acceleration due to gravity, n_i and λ_i are the unit vectors in the directions ox_3 and $o'x'_3$ respectively, δ_{ij} is the Kronecker delta and ϵ_{ijk} is the permutation tensor.

The last term in the right hand side of Equation (2.1) represents the 'Coriolis force' and the term before this is the 'centrifugal force'. Henceforth the latter terms will be combined with the gravitational term $\rho g n_i$ to give a resultant force which, because of the (non-spherical) shape of the earth's surface, is approximately normal to it (Barry et al. (1945)).

Mass conservation. The mass continuity equation takes the form

$$\rho_{,t} + (\rho U_j)_{,j} = 0 \quad (2.2)$$

Energy conservation. The equation describing the conservation of energy when radiative, and other sources of thermal energy are neglected (c.f. Bird et al. (1960)) can be written as

$$\rho c_v (\theta_{,t} + U_j \theta_{,j}) = (k_\theta \theta_{,i})_{,i} - \theta \left(\frac{\partial P}{\partial \theta} \right)_\rho U_{i,i} + \mu S \quad (2.3)$$

where: θ is the absolute temperature, c_v is the heat capacity of the fluid at constant volume and k_θ is the molecular thermal conductivity. The term μS represents energy generation due to viscous dissipation. As Spiegel and Veronis (1960) point out, the ratio of this term to the convection term $\rho c_v U_j \theta_{,j}$, is of the order $U l_k / v_k L$ where l_k , v_k are the mean free path and molecular velocity respectively and U and L are macroscopic velocity and length scales: therefore it plays an insignificant role in atmospheric application, and may be neglected.

Equation of state. The atmosphere will be assumed to act as an ideal gas, for which the equation of state is

$$P = \rho R \theta \quad (2.4)$$

where R here is the gas constant.

Conservation of pollutant species. Assuming Fick's law of diffusion to apply and in the existence of sources or sinks of the species considered due for example to chemical reaction, the equation expressing the conservation of a chemical species is (c.f. Csanady (1973):

$$C_{,t} + (U_i C)_{,i} = (\gamma_c C_{,i})_{,i} + S_c \quad (2.5)$$

where γ_c is the molecular diffusivity and S_c is any source of the species considered.

2.2 The Boussinesq approximation

Before any further manipulations on equations (2.1), (2.2), (2.3) and (2.5) are made they will first be transformed to the Boussinesq equations for shallow convection. Within the Boussinesq approximation the flow is assumed to behave as an incompressible flow with the temperature dependence of the density only taken into account when gravitational forces are considered. In the following paragraphs the conditions for which the Boussinesq approximation is justified will be outlined. Further details are given by Spiegel and Veronis (1960) and Calder (1968).

It is assumed that any variable ϕ , which may be P , θ or ρ can be decomposed into a value ϕ_m which is independent of height (normally taken as the ground value - see Calder (1968)), a value ϕ_o representing the variation of ϕ with height in the absence of fluid motion (i.e. the hydrostatic case) and a value γ which is the deviation of ϕ from the equilibrium condition in the presence of motion i.e.:

$$\phi = \phi_m + \phi_o + \gamma \quad (2.6)$$

If a height scale h_ϕ is defined as

$$h_\phi = \left| \frac{1}{\phi_m} \frac{\partial \phi_o}{\partial x_3} \right|^{-1} \quad (2.7)$$

then the Boussinesq approximation holds if for a convective layer of height δ

$$\frac{\delta}{h_\phi} = e \ll 1 \quad (2.8)$$

and

$$\left| \frac{\partial \phi}{\partial x_m} \right| \sim e \quad (2.9)$$

where $\sim$ indicates that the left hand term is the same order of magnitude as the right hand term. If the above conditions apply, equations (2.1) and (2.2) can be written, to order of magnitude e , respectively as:

$$U_{i,t} + U_j U_{i,j} = - \frac{1}{\rho_m} \bar{p}_{,i} + \beta_i \bar{\theta} + \nu U_{i,jj} + \alpha_{ik} U_k \quad (2.10)$$

$$U_{i,i} = 0 \quad (2.11)$$

where: $\beta_i \equiv g n_i / \theta_m$ and $\alpha_{ik} = -2\Omega \epsilon_{ijk} e_{sj} \lambda_s$

If further the gradient of θ_0 with x_3 is chosen equal to the adiabatic lapse rate, equation (2.3) then becomes:

$$\rho c_p (\bar{\theta}_{,t} + U_j \bar{\theta}_{,j}) = (k_\phi \bar{\theta}_{,j})_{,j} \quad (2.12)$$

where c_p is the thermal capacity of the fluid at constant pressure.

It should be mentioned that in the above analysis it is assumed that in the case of pollutant dispersal the flow field is not influenced by the existence of the contaminant, which is reasonable provided either the densities of the air and the contaminant are nearly equal or the concen-

tration of the contaminant is very small. A further consequence of this assumption in equation (2.5) is that C can be considered as either the density of the pollutant in the mixture or the mass fraction or volume fraction of the pollutant.

2.3 The averaged equations

Equations (2.5), (2.10), (2.11) and (2.12) if solved will give the instantaneous values of the variables throughout the spatial domain considered. Two main problems, however, arise in attempting to obtain such solutions. The first is in connection with imposing boundary and initial conditions because of the random nature of turbulence this is difficult except at ground level where the flow ceases to be turbulent. The second difficulty is that important features of turbulence can be of very small (compared to the dimensions of the solution domain) temporal and spatial scales; in atmospheric applications these scales can reach orders of one tenth of a second and one millimetre respectively. Now to adequately describe such features, in a numerical solution procedure that will be of any practical importance, will require a prohibitive amount of computer storage and time.

In order to overcome these problems the instantaneous equations are 'smoothed' out by an ensemble averaging process. Following this practice and assuming constant molecular properties Equations (2.5), (2.10), (2.11) and

(2.12) become*:

$$\bar{c}_{,t} + (\bar{u}_i \bar{c})_{,i} = - (\overline{u_i c})_{,i} + (\gamma_c \bar{c}_{,i})_{,i} + \bar{S}_c \quad (2.13)$$

$$\begin{aligned} \bar{u}_{,t} + (\bar{u}_i \bar{u}_j)_{,j} = & - \frac{1}{\rho} \bar{P}_{,i} + \beta_i \bar{\theta} - (\overline{u_i u_j})_{,j} \\ & + \nu \bar{u}_{i,jj} + \alpha_{ik} \bar{u}_k \end{aligned} \quad (2.14)$$

$$\bar{u}_{i,i} = 0 \quad (2.15)$$

$$\bar{\theta}_{,t} + (\bar{u}_j \bar{\theta})_{,j} = - (\overline{u_j \theta})_{,j} + (\gamma_\theta \bar{\theta}_{,j})_{,j} \quad (2.16)$$

where θ is the fluctuating temperature, $\gamma_\phi \equiv k_\theta / \rho c_p$ and $\overline{u_i c}$, $\overline{u_i u_j}$ and $\overline{u_j \theta}$ are turbulent fluxes of concentration momentum and heat respectively and are discussed in the following chapter.

2.4 Further simplifications

In general all the terms in the above equations may be important, depending on the location in the atmospheric layer, the time considered (day or night, summer, winter etc.), the boundary conditions etc. However further restrictions must be imposed in order to reduce the equations to a set which is more economical to solve.

*The suffix m and the tildas are omitted from ρ , P and θ respectively as we have no further occasion to refer to total values (of ϕ , see Equation (2.6)).

The first major restriction is that for the conditions of interest; the flow in the atmospheric layer will be assumed to obey the boundary layer approximations, which in simple terms entail that variations in the dependent variables, in the direction of flow are much less than those in the cross-stream directions. Hence if L_1 is a scale in the direction of flow and L_3 is the scale in the vertical direction then it follows that under these conditions:

$$\frac{\partial/\partial x_1}{\partial/\partial x_3} \sim L_3/L_1 \ll 1 \quad (2.17)$$

Furthermore only the mean concentration field will be allowed to be three dimensional and hence the velocity and temperature fields are assumed two dimensional ($\bar{U}_i$ and $\bar{\theta}$ varying only with x_1 and x_3).

It is clear that application of the boundary layer approximation prevents atmospheric conditions such as weak winds, strong convection currents ('thermals') and separation provoked by uneven topography to be examined within this framework.

With the above stated assumptions an order of magnitude analysis is next applied to the averaged equation listed below in order to assess the importance of the terms appearing in these equations.

Momentum conservation equations. From Equation (2.14) the stream-wise, lateral and vertical components of the velocity vector are governed, respectively, by the following equations

$$\begin{aligned} \bar{U}_{1,t} + \bar{U}_1 \bar{U}_{1,1} + \bar{U}_3 \bar{U}_{1,3} = & -\frac{1}{\rho} P_{,1} - (\overline{u_1 u_3})_{,3} + \nu \bar{U}_{1,33} \\ & - 2\Omega(e_{32} \bar{U}_3 - e_{33} \bar{U}_2) \end{aligned} \quad (2.18)$$

$$\begin{aligned} \bar{U}_{2,t} + \bar{U}_1 \bar{U}_{2,1} + \bar{U}_3 \bar{U}_{2,3} = & -\frac{1}{\rho} P_{,2} - (\overline{u_2 u_3})_{,3} + \nu \bar{U}_{2,33} \\ & - 2\Omega(e_{33} \bar{U}_1 - e_{31} \bar{U}_3) \end{aligned} \quad (2.19)$$

$$\begin{aligned} \bar{U}_{3,t} + \bar{U}_1 \bar{U}_{3,1} + \bar{U}_3 \bar{U}_{3,3} = & -\frac{1}{\rho} P_{,3} - (\overline{u_3 u_3})_{,3} + \nu \bar{U}_{3,33} + \beta_3 \bar{\theta} \\ & - 2\Omega(e_{31} \bar{U}_2 - e_{32} \bar{U}_1) \end{aligned} \quad (2.20)$$

Here the gradients of the turbulent and molecular fluxes in the streamwise direction have been neglected by virtue of (2.17), and all gradients in the lateral direction have been set to zero.

If it is assumed that:

$$U_{1,3} \sim W/L_3 \quad (2.21)$$

where W is a mean velocity scale; then from relation (2.17):

$$U_{1,1} \sim W/L_1 \quad (2.22)$$

and from the continuity Equation (2.15)

$$\bar{U}_3 \sim WL_3/L_1 \quad (2.23)$$

Now considering the equation of the streamwise component $\bar{U}_1$,

the order of magnitude of the pressure gradient term there can be obtained by integrating Equation (2.20) with respect to x_3 and then differentiating with respect to x_1 . If $(\int \beta_3 \bar{\theta} dx_3)^*_{,1}$ is neglected then it can be shown that

$$P_{,1} \sim P_{G,1} \quad (2.24)$$

where the subscript G refers to geostrophic conditions (other terms appearing are of the order L_3/L_1 times the inertia terms in (2.18)). The order of magnitude of the terms in Equation (2.18), in their order of appearance, can then be summarised as:

$$\frac{W}{T_m} \quad \frac{U_G W}{L_1} \quad \frac{W^2}{L_1} \sim f U_G \quad \frac{w^2}{L_3} \quad \frac{v W}{L_3} \quad f U_G \quad (2.25)$$

where U_G is the geostrophic velocity, w is a turbulence velocity scale, T_m is a time scale of the mean motion and $f \equiv 2\Omega e_{33}$ (for a non-accelerating geostrophic layer $\frac{1}{\rho} P_{G,1} \sim f U_G$). If all terms are compared to the convection term $\bar{U}_1 \bar{U}_{1,1}$ which is of the order $U_G W/L_1$ then (2.25) becomes:

$$\frac{L_1}{T_m U_G} \quad 1 \quad \frac{W}{U_G} \quad \sim \quad \frac{f L_3 L_1}{W L_3} \quad \frac{L_1 w^2}{L_3 U_G W} \quad \dots \quad \frac{L_1 \gamma}{L_3 L_3 U_G} \quad \frac{L_1 f L_3}{L_3 W} \quad (2.26)$$

*It is such terms that are responsible for macroscale motion.

The scales chosen for W , w and L_3 are respectively U_G , u_* and the planetary boundary layer thickness[‡] δ . Consequently it can be seen, from Equation (2.26), that compared to the convection term, the molecular term will be inversely proportional to the Reynolds number Re_δ ($\equiv U_G \delta / \nu$) which is normally much greater than L_1/L_3 and therefore, apart from a very thin region close to the ground (for rough surfaces this region does not exist at all) this term can be neglected.

For a typical value of U_G/u_* of 30 (c.f. Tennekes and Lumley (1974)) and assuming*

$$\frac{L_1}{L_3} \sim 1000 \quad (2.27)$$

which is quite adequate for a boundary layer assumption, then the ratio between the turbulent diffusion term $((\overline{u_1 u_3})_{,3})$ and the convection term is of the order

$$\frac{u_*^2}{\overline{U}_G^2} \frac{L_1}{L_3} \approx 1 \quad (2.28)$$

The relative importance of the pressure and Coriolis terms is measured by the ratio between L_1/L_3 and the Rossby number Ro_δ ($\equiv f\delta/U_G$). Assuming a boundary layer thickness of 500 m and a geostrophic wind velocity of 10 m/s then at a

[‡] This choice of scales could be a crude approximation for some of the regions in the planetary boundary layer considered.

* L_1/L_3 can vary over a wide range depending on factors such as topography, stratification etc.

latitude of 30° we get

$$\frac{f\delta}{\bar{U}_G} \frac{L_1}{L_3} \approx 4 \quad (2.29)$$

From relation (2.28) and (2.29), it is seen that the pressure, Coriolis, turbulent diffusion terms are approximately of the same order of magnitude as the convection term. For larger values of L_1/L_3 (assuming all other parameters constant) the former terms become dominant and the convection terms can be neglected.[‡]

When the flow in the atmospheric layer is similar*, the absolute value of the 'forces' on the right hand side of Equation (2.18) are rather small, in the sense that they tend to produce changes in momentum over relatively large distances; for example by employing the previous values of L_3 , L_1/L_3 etc. a variation of 100% in the velocity would occur over a distance of 500 km. Over shorter distances (up to about 20 km) we then expect an insignificant variation (of the order of 4%) in the mean velocity and thus from a practical point of view solution of the momentum equation is unjustified.

If, on the other hand, the flow experiences abrupt changes in boundary conditions, as for example, due to

[‡]In which case the velocity field becomes one dimensional.

*i.e. when, $(U_G - \bar{U}_1)/u_*$ is independent of x_1 . It is of course noted that complete similarity in the sense given by Hinze (1975) is not expected to hold.

sudden changes in ground roughness the Coriolis and Pressure forces (the latter, for regions away from the protuberances) are not largely affected however the convection and turbulent diffusion terms become large (L_1 and $L_3^\pm$ decrease) and a drastic change in the velocity profile can occur, even over short distances.

Because, in the present study, we are primarily interested in short range dispersal problems, the turbulent diffusion and convection are the only* terms that need concern us here. If we further neglect the unsteady term, then the streamwise velocity component will be governed by:

$$\bar{U}_1 \bar{U}_{1,1} + \bar{U}_3 \bar{U}_{1,3} = - (\overline{u_1 u_3})_{,3} \quad (2.30)$$

Considering next the lateral velocity $\bar{U}_2$, this is zero at ground level and is generally small up to heights of about 100 m (Panofsky (1973)). $\bar{U}_2$ is therefore neglected and Equation (2.19) will be considered no further.

According to Equation (2.25), $\bar{U}_3$ has a small value, however it is required for the solution of Equation (2.30). For the purpose of calculating $\bar{U}_3$ the continuity Equation (2.15)

$$\bar{U}_{1,1} + \bar{U}_{3,3} = 0 \quad (2.31)$$

will be used.

$^\pm L_3$ is no more taken as δ but more appropriately the disturbed region by the roughness elements.

*The importance of the unsteady term ($\partial/\partial t$) is discussed in Section 2.5.

Energy conservation. By neglecting the gradients of the molecular and turbulent fluxes in the streamwise direction (compared to those in the vertical direction) and also from the assumption of the two dimensionality of the temperature field we have from Equation (2.16)

$$\bar{\theta}_{,t} + \bar{u}_1 \bar{\theta}_{,1} + \bar{u}_3 \bar{\theta}_{,3} = - (\overline{u_3 \theta})_{,3} - (\gamma_\theta \bar{\theta}_{,3})_{,3} \quad (2.32)$$

$$\frac{L_1}{T_m U_G} \quad 1 \quad 1 \quad \frac{u_* \theta_* L_1}{U_G \Delta \theta L_3} \quad \frac{\gamma_\theta L_1}{\delta U_G L_3}$$

The relative order of magnitude of the terms are shown below the corresponding terms*. Where $\Delta \theta$ is the difference in $\bar{\theta}$ in a vertical distance of the order L_3 and θ_* is defined for a heat flux H at ground level, as:

$$\theta_* \equiv -H/\rho c_p u_* \quad (2.33)$$

It is apparent from (2.32) that the molecular term $\gamma_\theta \bar{\theta}_{,3}$ is negligible since the Pecklet number $Pe_\delta (\equiv \delta U_G/\gamma_\theta)$ is normally much greater than L_1/L_3 . Neglecting $\bar{\theta}_{,t}$ the energy Equation (2.32) then reduces to[‡]

$$\bar{u}_1 \bar{\theta}_{,1} + \bar{u}_3 \bar{\theta}_{,3} = - (\overline{u_3 \theta})_{,3} \quad (2.34)$$

*Generally speaking T_m , L_1 and L_3 can differ from those chosen for the analysis of the momentum equation however it is the ratio between them that interests us here.

‡This equation can also be employed to describe the variation of the potential temperature (Seinfeld (1975)).

Conservation of pollutant species. With similar assumptions to those applied to the momentum and energy equation, the conservation equation of the pollutant species can be written as:

$$\bar{U}_1 \bar{C}_{,1} + \bar{U}_3 \bar{C}_{,3} = -(\overline{u_3 c})_{,3} - (\overline{u_2 c})_{,2} + \bar{S}_c \quad (2.35)$$

It should be noted that variation of $\bar{C}$ with time is assumed to be wholly due to variations in the velocity field i.e. the source of pollutant is assumed to be continuous, or at least varies with a time scale much larger than that of the velocity field.

2.5 Averaging Process

Two types of averaging processes are generally considered in connection with atmospheric applications, namely ensemble averaging and time averaging (e.g. Lumley and Panofsky (1964)). These may be defined respectively as

$$\bar{\Phi} = \int_{-\infty}^{\infty} P(\Phi) \Phi d\Phi \quad (2.36)$$

$$\bar{\Phi}_T = \frac{1}{T} \int_t^{t+T} \Phi dt \quad (2.37)$$

where $\bar{\Phi}$ is the ensemble or 'probability mean' and $\bar{\Phi}_T$ is the time average of Φ over time T .

Forming an ensemble is equivalent to carrying out an experiment a large number of times, under the same conditions, in such a manner that the outcomes from every observation are statistically independent. Time averages, on the other hand, are obtained from a single experiment which is observed continuously for a time T .

In stationary flows the two averaging processes become equal provided that firstly the auto-correlation

$S_\phi(\xi)$ (where $S_\phi(\xi) \equiv \overline{\phi(t)\phi(t+\xi)}$) satisfies the condition

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T S_\phi(\xi) d\xi = 0 \quad (2.38)$$

and secondly that the averaging time (or 'sampling time' as referred to by meteorologists) is much greater than the Eulerian time scale Λ_E defined as:

$$\Lambda_E = \frac{1}{S_\phi(0)} \int_0^\infty S_\phi(\xi) d\xi \quad (2.39)$$

when the averaging time is not sufficiently larger than Λ_E then the variance of the difference between $\bar{\phi}$ and $\bar{\phi}_T$ is given by (c.f. Monin and Yaglom (1977)):

$$|\bar{\phi}_T - \bar{\phi}|^2 \approx 2 \frac{\Lambda_E}{T} S_\phi(0) \quad (2.40)$$

In the atmosphere the flow is not stationary and the integral scales, if they exist, are expected to be very large. This will lead to a situation where, if time averages are applied then the resultant mean values are bound to be functions of the averaging time and also of the chosen time origin.

If theoretically speaking, T is extended to infinity then $\overline{\Phi}_T$ will tend to a constant value that is different from $\overline{\Phi}$ (as only the latter will vary with time). Thus the two averages are not expected to be equal in atmospheric applications.

Although ensemble averaging is the obvious method to apply when studying unsteady processes it is very time-consuming and expensive to perform experimentally when atmospheric plume dispersal is considered. Thus in the majority of continuous plume measurements time averages are employed (c.f. Slade (1968)).

Of particular interest in connection with plume behaviour is the effect of averaging time on the diffusion parameter σ_2 (the lateral dispersal parameter) and the maximum concentration C_m . Experimental evidence, as demonstrated by the summary given by Hino (1968), indicates that as the sampling time is increased σ_2 continuously increases (σ_3 also initially increases slightly, then tends to a constant value) with consequential reduction in C_m . This phenomenon can be explained as follows: for small averaging times T , the statistical influence of the large scale motion on the diffusion is negligible; however as T is increased the diffusion becomes more and more affected statistically, by the large eddies. In effect, in taking large averaging times the effects of both the spread of the plume about its instantaneous axis (which can be considered as a relative diffusion process, see for example Csanady (1973)) and the meandering of the plume, intact, about the mean wind direction are superimposed.

In practice it is desirable to consider both short and long time averages, because the former would give the minimum spreading rate and hence the highest concentration levels while the latter would yield the maximum area contaminated. A schematic diagram of the effect of the averaging time on averaged concentration profile is shown in Figure 2.2.

For reasons mentioned, in the present analysis time averages will be employed and instantaneous values are therefore replaced by:

$$\phi = \bar{\phi}_T + \phi \quad (2.41)$$

It is seen from Equation (2.41) that because $\bar{\phi}_T$ depends on the averaging time T , then ϕ will also depend on T ; or in other words the averaging time will be an influential factor in deciding how much of ϕ is ascribed to mean motion and how much to 'turbulence'. It must be added, however, that the choice of the value of T is not arbitrary but must be made in view of the following considerations.

(i) Although more information can be gained by reduction* of T , it cannot be reduced indefinitely. Otherwise the averaged equations would tend to the instantaneous ones, which for reasons noted earlier is undesirable. A compromise must therefore be sought.

(ii) In the derivation of the averaged equations it is implicitly assumed that the averaging process satisfies, what Kamp de Fériet (1951) defines as, Reynolds axioms:

*Theoretically speaking if $T \rightarrow 0$ then all the 'turbulence signal' is available and for a long enough signal all moments can then be calculated.

$$\overline{F + G} = \overline{F} + \overline{G} \quad (2.42)$$

$$\overline{aF} = a\overline{F} \quad (2.43)$$

$$\frac{\partial \overline{F}}{\partial s} = \frac{\partial}{\partial s} \overline{F} \quad (2.44)$$

$$\overline{FG} = \overline{F} \overline{G} \quad (2.45)$$

where: F and G are any instantaneous variables, a is a constant and s is either x_1 or t. When time averages are employed Equation (2.42), (2.43) and (2.44) are readily satisfied, however axiom (2.45) can only be (approximately) satisfied if the averaging period T be large in comparison with the characteristic periods of the fluctuating quantity g (where g is the fluctuating component of G) but small in comparison to the time scale of $\overline{F}$ (c.f. Monin and Yaglom (1977)). In atmospheric application this latter condition could be partially fulfilled as expounded in the following discussion.

Figure 2.3 shows a typical horizontal wind speed spectrum given by Van Der Hoven (1957). It is seen that energy is concentrated about the two major frequencies of 10^{-2} cycles/h and 50 cycles/h with a 'spectral gap' separating these two. The lower frequency is concentrated about the synoptic weather map scales while the high frequency corresponds to micrometeorological scale. Van Der Hoven (1957) attributes the existence of the gap, to the lack of sources of energy, that could support the fluctuations in this frequency range.

Now, if we were to treat all fluctuations in the micro-meteorological scale as turbulence we would require according to Figure 2.3, an averaging time of about 20 minutes*. By neglecting the energy in the spectral gap then the time scale of $\overline{F^\ddagger}$ would be at least of the order of 4 hours i.e. about 12 times as large as T. Under such conditions Reynolds' axiom (2.45) could then be approximately fulfilled.

It should be added that if any of the variables (U_i , θ ... etc.) has large amounts of energy in the region of the gap then obviously the above argument is weakened.

Because some of the important features of plumes (e.g. σ_2) change by increasing the averaging time, a method is given in Appendix B1 by which long time-averaged plumes can be 'extrapolated' from short time averaged data.

From the previous discussion we concluded that the time scale of the averaged quantities is about 4 hours, hence the unsteady terms ($\partial/\partial t$) appearing in Equations (2.13), (2.14) and (2.16) would have the same order of magnitude as the convection term ($\overline{U}_j \partial/\partial x_j$) if:

$$L_1 \sim T_m U_G = 144 \text{ km}$$

If L_1 is assumed much smaller than this value, then the unsteady terms could be neglected.

*Which is greater than the characterisitic frequency in the micrometeorological range.

$\ddagger$ If F is time averaged, over T, all motions with frequencies much larger than $1/T$ are eliminated (averaging acts as a filter which eliminates high frequencies).

2.6 Summary of the equations

The averaged equation set that is to be solved in the present study comprises the continuity equation, the streamwise momentum conservation equation, the energy conservation equation and the conservation equation of the pollutant species considered. These are assumed to have the following forms*:

Continuity equation

$$\bar{U}_{1,1} + \bar{U}_{3,3} = 0 \quad (2.46)$$

Streamwise momentum equation

$$\bar{U}_1 \bar{U}_{1,1} + \bar{U}_3 \bar{U}_{1,3} = - (\overline{u_1 u_3})_{,3} \quad (2.47)$$

Energy equation

$$U_1 \bar{\theta}_{,1} + U_3 \bar{\theta}_{,3} = - (\overline{u_3 \theta})_{,3} \quad (2.48)$$

Pollutant concentration equation

$$\bar{U}_1 \bar{C}_{,1} + \bar{U}_3 \bar{C}_{,3} = - (\overline{u_2 c})_{,2} - (\overline{u_3 c})_{,3} + \bar{S}_c \quad (2.49)$$

Solution of Equations (2.46), (2.47), (2.48) and (2.49) is discussed in Chapter 4.

*The overbars without suffix T will henceforth indicate time averages.

CHAPTER 3

TURBULENCE MODEL

In this chapter the mathematical model proposed for the closure of the ensemble-averaged transport (2.47), (2.48) and (2.49) is presented. In section 3.1 the strategy and the order of closure are discussed; it is proposed there that transport equations for the unknown turbulence fluxes $\overline{u_i u_j}$, $\overline{u_i \theta}$ and $\overline{u_i c}$ should be solved together with equations for k and ϵ . These are presented in their 'exact form' in section 3.2 and are then, under certain assumptions, simplified. In section 3.3 the modelling of the various higher-order correlations appearing in the equations is discussed; starting with those relating to the hydrodynamics in 3.3.1 and 3.3.2, and proceeding in 3.3.3 to those for the turbulent scalar fluxes. Section 3.4 describes a procedure (due to Launder (1976) and Rodi (1972)) by which the differential transport equations of the turbulent fluxes may be simplified to algebraic form, under certain assumptions. This approach is employed here in order to reduce the number of partial differential equations required to be solved.

It should be stated that although the proposed closure is intended to be nominally a second order (i.e. where transport equations of second order moments are considered) nonetheless classical mixing-length concepts are implicitly or explicitly employed on occasions. This is done, as will be explained, in part to avoid mathematical difficulties and also in a quest for simplicity and hence economy.

3.1 Closure procedure

As mentioned earlier, to solve the mean flow equations it is necessary to relate the unknown correlations (e.g. $\overline{u_i u_j}$, $\overline{u_i \theta}$ etc.) to known or calculable quantities.

Ideally the relationship would be a versatile relation that defines the fluxes in terms of known local (in time and space) variables. Such a relationship does, for example, exist in laminar flows of Newtonian fluids, where the stress and strain tensors at a point are related by a constitutive law that is independent of the history of the straining action and of any particular conditions (such as boundary and initial conditions) of the flow situation. This behaviour is possible because of the decoupling between the mean and molecular motions.

Unfortunately such a decoupling does not, generally, exist in turbulent flows, which exhibit strong interactions between the mean motion and turbulence. Unlike molecular motion turbulence depends on the mean strain rate (in the absence of buoyancy and other forms of energy) for its existence and thus cannot be regarded as having intrinsic properties that would enable it to respond indifferently*to the mean field.

In view of the strong coupling between the turbulent and mean motions, the former acquires relatively long length

*For example, turbulence can in some instances behave as a viscous medium while in some others it responds as an elastic material, depending on how the mean strain is applied c.f. Crow (1968).

and time scales (memory) which make eddies 'remember' the straining action which they were previously subjected to. Therefore any relation linking turbulent quantities and the mean field should reflect this fact.

From ideas borrowed from continuum mechanics Lumley (1967) suggested that the turbulent stress at a point should be a functional of the mean deformation rate throughout the flow, with the statistics of the turbulent field acting as 'material constants'. The functional is then expanded in a series that has its terms corresponding to longer and longer (as Lumley puts it) 'memory' and 'awareness' of the turbulent field. By assuming limited awareness and a fading memory the series could then be truncated after a finite number of terms. Such a procedure seems plausible however to be of practical utility the turbulence must have a relatively short time and length scale.

The evolution of the turbulent fluxes could, alternatively, be exactly described by a dynamic equation rigorously derived from the instantaneous equations of momentum, energy etc. (e.g. Chou (1945)). These derived equations, however, contain additional unknowns in the form of third order correlations for which further equations must be found: these can also be generated, but turn out to contain still higher order correlations, and so on. In general the number of equations generated by this approach will always be one less than the number of unknown correlations. In addition an ever increasing number of defining scalars will be required for each order of correlations so that the number of equations and terms apparently increases indefinitely.

Batchelor (1959) pointed out however that the process of generating equations for higher order correlations need not go on indefinitely if the turbulence can statistically be represented by a large but finite number of equations. The unknown correlations could then, under certain assumptions be written in terms of lower order moments.

The rationale behind this procedure is that it is reasonable to expect that if the equations for lower order moments are considered in their complete form, and assumptions are made only to equations of higher order moments, then the lower order moments will be less sensitive to the assumptions. Obviously some drawbacks exist in increasing the level of closure these can be summed as:

- (i) Modelling of terms in the higher order equations demands measurements and physical understanding which become more difficult as the order increases.
- (ii) The amount of computational effort becomes excessive.

A compromise between complexity and accuracy should thus be sought. In the present formulation transport equations are assembled for, non-zero components, of the second order moments $\overline{u_i u_j}$, $\overline{u_i c}$ and $\overline{u_i \theta}$ together with the dissipation rate $\epsilon (\equiv \nu \overline{(u_{i,j})^2})$. The latter represents the dissipation rate in the turbulence kinetic energy equation and also together with $k (\equiv \overline{u_i^2}/2)$ defines a time (or length scale for the turbulent motion.

It should be added, that solution of the equations for the correlations, $\overline{c^2}$ and its dissipation rate $\epsilon_c (\equiv \gamma \overline{(c_{,i})^2})$ would have been useful to the present analysis; this is because the ratio $\overline{c^2}/\epsilon_c$ provides a time scale for the concentration field which, as will be seen, plays an important role in the modelling of the equation for $\overline{u_i c}$, and also,

knowledge of $\bar{c}^2$ is in itself useful as it gives an indication of the deviation of the concentration from its mean value. However the modelling of the equation of ϵ_c is still in the developing stage (initial suggestions are given by Lumley and Khajeh-Nouri (1974) also discussed by Launder (1976)); moreover for three dimensional concentration fields $\bar{c}^2$ and ϵ_c are three dimensional, solving their equations would add a great deal to the computer time and storage required.

3.2 Turbulence equations

3.2.1 The equations for the Reynolds stresses and turbulence energy

The exact equations for the transport of the Reynolds stress tensor ($\overline{u_i u_j}$) can be derived from equation (2.1). Gence (1977), however, has shown that the equation for $\overline{u_i u_j}$ can be derived, to a certain degree of approximation from the Boussinesq equation* (2.10) provided the following conditions are fulfilled:[‡]

$$O \left\{ \nu \left(\frac{1}{3} \overline{u_{k,ik}} + \overline{u_{i,kk}} \right) \right\} < g \quad (3.1a)$$

*The Boussinesq equation leads to a much simpler equation for $\overline{u_i u_j}$ than if equation (2.1) is used.

[‡]The notation $O \{ \quad \}$ here signifies the order of magnitude of the bracketed quantity.

$$O \{ \bar{P}_{,i} / \rho \} < g \quad (3.1b)$$

$$O \{ \bar{\theta} \} < \theta' / Fr_L, \quad (3.1c)$$

$$Fr_L, < 1 \quad (3.1d)$$

$$O \{ \bar{\theta}_{,i} \} < L' \theta' g / \nu u' \quad (3.1e)$$

Where: $\theta' \equiv \sqrt{\bar{\theta}^2}$, $u' \equiv \sqrt{\bar{u}_i^2}$, L' is an integral length scale and $Fr_L,$ is the turbulent Froude number defined by: $Fr_L, \equiv u'^2 / g L'$. By noting that L' is roughly of the order of the boundary layer thickness and $\theta' \sim \theta_*$; and by following arguments given in section 2.4, conditions (3.1a) to (3.1e) could consecutively be reformulated as:

$$O \{ \frac{\nu U_G}{\delta^2 g} \} < 1 \quad (3.2a)$$

$$O \{ \frac{f U_G}{g} \} < 1 \quad (3.2b)$$

$$O \{ \theta_* / \bar{\theta} \} > \{ u_*^2 / g \delta \} \quad (3.2c)$$

$$O \{ \frac{u_*^2}{g \delta} \} < 1 \quad (3.2d)$$

$$O \{ \theta_* / \Delta \theta \} > O \{ \frac{\nu u_*}{\delta^2 g} \} \quad (3.2e)$$

where $\Delta\theta$ is the change in $\bar{\theta}$ across a vertical distance L' .

For typical values, in atmospheric applications, of:
 $U_G \sim 10$ m/s, $u_* \sim 0.2$ m/s, $\delta \sim 500$ m, $\theta_* \sim 0.15^\circ\text{K}$, $\bar{\theta} \sim \Delta\theta \sim 3^\circ\text{K}$;
 it could be seen that conditions (3.2) are easily satisfied.
 Thus an equation for u_i can be derived by subtracting the
 time-averaged Boussinesq equation (2.14) from the instant-
 aneous version (2.10), yielding:

$$u_{i,t} + \bar{u}_j u_{i,j} = -u_j \bar{u}_{i,j} - u_j u_{i,j} + \overline{u_j u_{i,j}} - \frac{1}{\rho} p_{,i} + \beta_i \bar{\theta} + \nu u_{i,kk} + \alpha_{ik} u_k \quad (3.3)$$

Multiplication of equation (3.3) by u_j and addition of the
 same equations with suffixes i and j interchanged, then
 time-averaging the result as suggested in section 2.5 yields,
 after rearranging, the following equation for $\overline{u_i u_j}$:

$$\begin{aligned} & \text{I} \quad \quad \quad \text{II} \quad \quad \quad \text{III} \\ & (\overline{u_i u_j})_{,t} + \bar{u}_k (\overline{u_i u_j})_{,k} = -(\overline{u_i u_k} \bar{u}_{j,k} + \overline{u_j u_k} \bar{u}_{i,k}) \\ & \quad \quad \quad \text{IV} \quad \quad \quad \text{V} \quad \quad \quad \text{VI} \\ & + (\beta_i \bar{\theta} u_j + \beta_j \bar{\theta} u_i) - 2\nu \overline{u_{i,k} u_{j,k}} - (\overline{u_i u_j u_k} - \nu (\overline{u_i u_j})_{,k} \\ & \quad \quad \quad \text{VII} \\ & + \frac{\bar{p}}{\rho} (\delta_{kj} u_i + \delta_{ki} u_j))_{,k} + \frac{\bar{p}}{\rho} (u_{i,j} + u_{j,i}) \\ & \quad \quad \quad \text{VIII} \\ & + (\alpha_{ik} \overline{u_k u_j} + \alpha_{jk} \overline{u_k u_i}) \end{aligned} \quad (3.4)$$

Setting $j = i$ and contracting over i gives the trace of the
 Reynolds stress tensor which when divided by 2 gives the
 following equation for the turbulence kinetic energy $k \equiv \overline{u_i u_i}/2$:

$$\begin{array}{ccccc}
 \text{I} & \text{II} & \text{III} & \text{IV} & \text{V} \\
 k_{,t} + \bar{U}_k k_{,k} = -\bar{u}_i \bar{u}_j \bar{U}_{i,j} + \beta_j \bar{\theta} \bar{u}_j - \overline{v(u_{i,j})^2} \\
 & & \text{VI} & & \\
 - \left(\frac{\overline{u_j u_i^2}}{2} - \nu k_{,j} + \frac{\overline{\theta u_j}}{\rho} \right)_{,j} & & & &
 \end{array} \quad (3.5)$$

The various terms in (3.4) and (3.5) can be associated with the following physical processes

Term I $\equiv$ temporal change

Term II $\equiv$ 'convection' by the action of mean motion

Term III $\equiv$ 'production' of $\overline{u_i u_j}$ or k by interaction of turbulence with mean-strain (often called 'mechanical production')

Term IV $\equiv$ 'production/destruction' (depending on the sign of the turbulent heat flux $\overline{u_j \theta}$) due to thermal stratification

Terms VI $\equiv$ 'diffusion' by respectively the actions of turbulence, viscosity and fluctuating pressure. An important characteristic of the group of terms is that its integral across the boundary layer is zero.

Term VII $\equiv$ 'pressure-strain' mechanism which distributes energy among the different stress components but does not directly alter, for incompressible flow, the level of the turbulence intensity k . It acts as a sink of $\overline{u_i u_j}$ when $i \neq j$.

Term VIII $\equiv$ 'Coriolis redistribution' mechanism which also distributes energy between different components, because its trace is equal to zero, this term does not appear in the equation for k .

Although term VIII and the viscous diffusion parts of VI require no further modelling they may in any case be neglected because their order of magnitude compared to that

* Term V $\equiv$ destruction by molecular action

of the production term III is of the order of the reciprocal of the Rossby* and Reynolds numbers respectively. This leaves term V, VI and VII in equation (3.4) and VI in equation (3.5) to be modelled: the practices adopted are described later in Section 3.3.1.

3.2.2 Transport equation for the dissipation rate

In the literature the dissipation rate of turbulence kinetic energy is usually defined as (Hinze (1975))

$$\epsilon = \overline{v s_{ij} s_{ij}} \quad (3.6)$$

where s_{ij} here is the fluctuating strain rate tensor

$$s_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

In equation (3.5) the dissipation rate implied is

$$\epsilon = \overline{v (u_{i,j})^2} \quad (3.7)$$

The choice between the two definitions (3.6) and (3.7) for ϵ depends upon the form of the viscous diffusion term adopted; if the dissipation rate is defined by (3.6) then the viscous diffusion terms appearing in equation (3.5) should be replaced by $2\overline{v(u_i s_{ij})_{,j}}$. In either case, as is shown in Appendix C1, for high turbulence Reynolds numbers $\overline{u_{j,i} u_{i,j}}$ is much smaller than $\overline{(u_{i,j})^2}$ (for $i \neq j$) and thus

*Typically of the order 10^3 .

$$\overline{v(u_{i,j})^2} \approx \overline{v s_{ij} s_{ij}} = \epsilon$$

An equation for ϵ (as defined by (3.7)) can be derived by differentiating equation (3.3) with respect to x_1 and multiplying the resultant by $2v u_{i,1}$ then time averaging; with some manipulation the following result is arrived at (for details see Reece (1977)):

$$\begin{aligned} & \begin{matrix} (i) & (ii) & (iii) & (iv) \end{matrix} \\ & \epsilon_{,t} + \overline{u_j \epsilon_{,j}} = -2v \overbrace{(u_{i,1} u_{j,1} + u_{1,i} u_{1,j})}^{(vi)} \overline{u_{i,j}} - 2v \overbrace{u_{i,j} u_{i,1} u_{j,1}}^{(vii)} \\ & \quad \quad \quad (v) \quad \quad \quad (vi) \quad \quad \quad (vii) \\ & - 2 \overbrace{(v u_{i,j,1})^2}^{(viii)} - v \overbrace{(u_j (u_{i,1})^2)_{,j}}^{(ix)} + 2 \frac{v}{\rho} \overbrace{(u_{i,1} p_{,1})_{,i}}^{(x)} \\ & \quad \quad \quad (viii) \quad \quad \quad (ix) \quad \quad \quad (x) \quad \quad \quad (xi) \\ & - 2v \overline{u_j u_{i,1} \overline{u_{i,1j}}} + v \epsilon_{,jj} + 2v \beta_{i,1} \overline{\theta u_{i,1}} + v \alpha_{ik} \overline{u_{k,1} u_{i,1}} \end{aligned} \quad (3.8)$$

Equation (3.8) in this form is virtually intractable, fortunately for larger turbulence Reynolds number many of the terms of (3.8) can be neglected as is next shown.

The order of magnitude of each of the terms in (3.8) can be evaluated in terms of the velocity and temperature scales u' and θ' together with the length scales l , λ and η . Here l is the length scale of the energy-containing eddies and is related to u' and ϵ by (Batchelor (1959))

$$l = A u'^3 / \epsilon \quad (3.9)$$

A being a constant of order unity. λ is the Taylor microscale defined as

$$\lambda = \sqrt{(u_{1,1})^2 / u_1^2}$$

in isotropic turbulence (c.f. Hinze (1975))

$$\lambda = \sqrt{15 \nu u'^2 / \epsilon} \quad (3.10)$$

The quantity η is the Kolmogorov microscale and is the smallest scale defined in turbulent motion, this is written as (c.f. Hinze (1975))

$$\eta = (\nu^3 / \epsilon)^{\frac{1}{4}} \quad (3.11)$$

Thus the relation among the length scales in isotropic turbulence is

$$\lambda / l = \left(\frac{15}{A} \right)^{\frac{1}{2}} Re_1^{-\frac{1}{2}} \quad (3.12)$$

$$\eta / l = A^{-\frac{1}{4}} Re_1^{-\frac{3}{4}} \quad (3.13)$$

$$\lambda / \eta = \left(\frac{225}{A} \right)^{\frac{1}{4}} Re_1^{\frac{1}{4}} \quad (3.14)$$

where Re_1 is the turbulence Reynolds number $u'l/\nu$.

It is shown in appendix C1 that the order of magnitude of each of the terms appearing in equation (3.8), non-dimensionalised with $\nu u'^3 / \lambda^3$ could be written as:

$$\text{Term (i)} \sim Re_1^{-\frac{1}{2}} \frac{1}{u'T}$$

$$\text{Term (ii)} \sim Re_1^{-\frac{1}{2}}$$

$$\text{Term (iii)} \sim \text{Re}_1^{-1}$$

$$\text{Term (iv)} \sim 1$$

$$\text{Term (v)} \sim 1$$

$$\text{Term (vi)} \sim \text{Re}_1^{-\frac{1}{2}}$$

$$\text{Term (vii)} \sim \text{Re}_1^{-1}$$

$$\text{Term (viii)} \sim \text{Re}_1^{-1.5}$$

$$\text{Term (ix)} \sim \text{Re}_1^{-1.5}$$

$$\text{Term (x)} \sim \text{Rf} \text{Re}_1^{-1}$$

$$\text{Term (xi)} \sim \text{Ro}_1^{-1} \text{Re}_1^{-\frac{1}{2}}$$

where Ro_1 is the turbulent Rossby number* based on l , i.e.

$$\text{Ro}_1 = \frac{u'}{f l}$$

and Rf is the flux Richardson number which is the ratio between production of k by buoyancy and mechanical production i.e.:

*In atmospheric application $\text{Ro}_1 \sim 40$.

$$Rf = \beta_m \frac{\overline{u_i \theta}}{\overline{u_i u_j} \overline{U}_{i,j}}$$

If all terms of order smaller than $Re_1^{-\frac{1}{2}}$ are neglected then equation (3.8) for ϵ reduces* to

$$\begin{array}{ccccc} \text{(a)} & \text{(b)} & \text{(c)} & \text{(d)} & \text{(e)} \\ \epsilon_{,t} + \overline{U}_j \epsilon_{,j} = & -2\nu \overline{u_{i,j} u_{i,1} u_{j,1}} & - 2(\overline{\nu u_{i,j1}})^2 & - \overline{\nu (u_j (u_{i,1})^2)}_{,j} \end{array} \quad (3.15)$$

The terms in (3.15) can be visualised as having the following physical meanings

Term (a) is a temporal change (or unsteady) term

Term (b) is the convection of ϵ by mean motion

Term (c) is the production of ϵ by vortex stretching action

Term (d) is the destruction of ϵ by viscous action (this term is always negative)

Term (e) is the diffusion of ϵ by turbulent motion

Apart from terms (a) and (b) all terms in (3.15) require to be modelled.

3.2.3 Turbulent heat flux equation

An exact equation for the scalar flux $\overline{u_i \theta}$ can be derived from equation (2.1) and (2.3), but as in the derivation of the Reynolds Stress equation Gence (1977) has shown that the Boussinesq equations (2.10) and (2.12) could be employed (these give a simpler equation for $\overline{u_i \theta}$) for this

*Term (a) (i.e. $\epsilon_{,t}$) is discussed further in sub-section 3.2.5.

purpose provided in addition to the restrictions (3.1a) to (3.1e) the following conditions are satisfied:

$$\frac{R}{\bar{C}_p} \frac{\theta_m}{\theta'} Fr_{L'} < 1 \quad (3.16a)$$

$$Ec_t Fr_{L'} \frac{\theta_m}{\theta'} < 1 \quad (3.16b)$$

$$O\{\bar{U}_{i,i}\} < \frac{\theta'}{\theta_m} \frac{1}{Ec_t} \frac{g}{u'} \quad (3.16c)$$

$$O\{\bar{\theta}_{,kk}\} < \frac{\theta'}{\lambda^2} \frac{1}{Fr_{L'}} \quad (3.16d)$$

$$O\{\bar{U}_{i,j}\} < \frac{\theta'}{\theta_m} \frac{1}{Ec_t} \frac{L'g}{v} \quad (3.16e)$$

where Ec_t is the turbulent Eckert number $u'^2/R\theta'$.

Typically in normal atmospheric conditions $\theta_m \sim 300^\circ K$ from values (of u' , θ' and L') quoted earlier $Fr_{L'} \sim 10^{-5}$ and $Ec_t \sim 10^{-2}$; using equation (3.12) we get $\lambda \sim 1 Re_1^{-0.5} \sim 0.2m$. Following a similar procedure as in section 2.4 and noting that the order of the dilatation $\bar{U}_{i,i}$ is less than 1 (see Spiegel and Veronis (1960)) it could be shown that conditions (3.16) are easily satisfied.

By multiplying the equation (2.12) by u_i , adding to it the x_i component of the Navier-Stokes equation (2.10) multiplied by θ and then time averaging the following transport equation for $\overline{u_i \theta}$ is obtained

$$\begin{aligned}
& \text{I} \quad \text{II} \quad \text{III} \quad \text{IV} \\
& (\overline{u_i \theta})_{,t} + \overline{u_j} (\overline{u_i \theta})_{,j} = -(\overline{u_i u_j \theta})_{,j} + \overline{u_j \theta} \overline{u_{i,j}} + \beta_i \overline{\theta^2} \\
& \quad \quad \quad \text{V} \quad \quad \quad \text{VI} \quad \quad \quad \text{VII} \\
& + (\nu + \gamma_\theta) \overline{\theta_{,j} u_{i,j}} + \frac{\overline{p \theta}}{\rho}_{,i} - (\overline{u_j u_i \theta} + \frac{\overline{p \theta} \delta_{ij}}{\rho} + \nu (\overline{u_i \theta})_{,j})_{,j} \\
& \quad \quad \quad \text{VIII} \\
& + \alpha_{ik} \overline{u_k \theta}
\end{aligned} \tag{3.17}$$

The various terms in the above have the following physical significance

Term I = Temporal change

Term II = Transport by mean motion

Term III = Generation by the interaction of the turbulence field with gradients in mean temperature and velocity respectively

Term IV = Production or dissipation by gravitational forces (depending on the sign of $\overline{u_i \theta}$)

Term V = Dissipation by viscous effects

Term VI = Pressure-temperature counterpart of the pressure strain term in the Reynold stress equation,

Term VII = Diffusion by turbulence, pressure and viscous effects

Term VIII = Production or destruction term by Coriolis forces

In view of the arguments given in appendix C1 term V is of the order

$$(v + \gamma_\theta) \overline{_{,j} u_{i,j}} \sim (v + \gamma_\theta) \frac{\theta u^i}{\lambda^2} \frac{\lambda}{1}$$

comparing this to the production term III (of order $u'^2\theta'/l$).

$$\text{term V / term III} \sim \text{Re}_\lambda^{-1} + \text{Pe}_\lambda^{-1}$$

Re_λ and Pe_λ are respectively the Reynolds and Pecklet numbers based on the length scale λ . Since for air the laminar Prandtl number is close to unity then

$$\text{Pe}_\lambda \approx \text{Re}_\lambda \sim \text{Re}_1^{\frac{1}{2}}$$

Therefore for high Reynolds number term V can be neglected. Though term VIII needs no further modelling it is neglected on the grounds that its order of magnitude compared to that of term III is of the order of the reciprocal of the Rossby number. Finally, by neglecting viscous diffusion ($\sim \text{Re}_1^{-1}$ times term III), the equation for the transport of $\overline{u_i \theta}$ reduces to

$$\begin{aligned} (\overline{u_i \theta})_{,t} + \overline{u_j} (\overline{u_i \theta})_{,j} = & -(\overline{u_i u_j \theta})_{,j} + \overline{u_j \theta} \overline{u_{i,j}} + \beta_i \overline{\theta^2} \\ & + \frac{\overline{p \theta}}{\rho}_{,i} - (\overline{u_j u_i \theta} + \frac{\overline{p \theta}}{\rho} \delta_{ij})_{,j} \end{aligned} \quad (3.18)$$

The terms requiring further attention are those describing gravitational effects, pressure-temperature interactions and diffusion. These will be considered later.

3.2.4 Transport equation for turbulent species flux

With a similar procedure to that leading to equation (3.18) yields the following equation for the turbulent flux of a chemical species $\overline{u_i c}$

$$\begin{aligned} (\overline{u_i c})_{,t} + U_j (\overline{u_i c})_{,j} = & - (\overline{u_i u_j c})_{,j} + \overline{u_j c} \overline{U_{i,j}} + \beta_i \overline{\theta c} \\ & + \frac{\overline{p c}}{\rho}_{,i} - (\overline{u_i u_j c} + \frac{\overline{p c} \delta_{ij}}{\rho})_{,j} \end{aligned} \quad (3.19)$$

whose terms have analogous significance to those of (3.18).

3.2.5 Temporal change terms

The relative importance (compared to the convection term) of the temporal change terms of the averaged correlations can be assessed by way of the value of the dimensionless parameter L_1/TU_G ; this was assumed in section 2.5 to be sufficiently small so as to be neglected. Hence all $\partial/\partial t$ terms appearing in all the turbulence equations considered will henceforth be dropped.

3.3 Closure of the turbulence equations

In order to close equations (3.4), (3.15), (3.18) and (3.19) it is necessary to link the unknown terms with other known quantities.

For this purpose Lumley extended his ideas regarding the modelling of second order terms mentioned in section 3.1 to higher order correlation (c.f. Lumley (1975), Lumley and Khajeh-Nouri (1974) also Siess (1975)). Briefly, Lumley suggests that third order terms can be expressed as functionals, over space and time, of variables of lower order moments (expressed in such a way that all tensors in the argument of the functional vanish in isotropic turbulence). The argument of the functional are then expanded in a Taylor series in time and space around the point being considered. With the assumption of weak inhomogeneity and short memory the series may be truncated, reducing the functional to a

local one. Next a tensor invariant form of the argument variable is constructed with coefficients being functions of invariants of the argument. Finally the latter are expanded around the isotropic condition; with the assumption of weak non-isotropy only lower order terms in the series are retained.

A less complex yet on some occasions (e.g. in wall flows) more practical procedure, was developed by Launder (1975) and Launder et al (1975). This procedure is adopted in the present investigation albeit with some modifications to the treatment of the equations for the turbulent concentration flux and the dissipation rate.

3.3.1 Reynolds stresses and turbulence energy

(a) Viscous destruction term: This term has its major energy contribution in the high wave number range of the energy spectrum for which, as discussed in sub-section 3.2.2, at high Reynolds number the turbulence is nearly isotropic and therefore (c.f. Hinze (1975))

$$\overline{v u_{i,k} u_{j,k}} = \frac{\varepsilon}{3} \delta_{ij} \quad (3.20)$$

(b) Diffusion term: The diffusion of $\overline{u_i u_j}$ has two components, one being the triple correlation $(\overline{u_k u_i u_j})_{,k}$ and the other the pressure velocity correlation $(\frac{p}{\rho} u_i)_{,j}$. The latter quantity has apparently never been measured and little is known about it, though it was suggested by Hanjalic and Launder (1972a) that in channel flows away from the vicinity of walls it is probably small.

Donaldson (1972) made the following proposition* for the modelling of the pressure-velocity correlations

$$\overline{\frac{pu}{\rho}}_i = c_d \sqrt{k} l_1 (\overline{u_i u_m})_{,m} \quad (3.21)$$

where c_d is some constant and l_1 is a turbulence length scale. No assessment can be made as regards the performance of (3.21) since no measurements of $\overline{\frac{pu}{\rho}}_i$ are available. In view of current lack of knowledge it will be neglected here.

Donaldson (1972) also suggested the following for the third-order velocity correlation:

$$\overline{u_i u_j u_k} = - l_1 \sqrt{k} ((\overline{u_j u_k})_{,i} + (\overline{u_i u_k})_{,j} + (\overline{u_i u_j})_{,k}) \quad (3.22)$$

This expression was chosen so as to satisfy the conditions of invariance (under arbitrary coordinate or Galilean transformation) and to possess the same tensor characteristics and dimensions as the original term.

Hanjalic and Launder (1972b) deduced the following alternative form for $\overline{u_i u_j u_k}$, from a truncation of its transport equation:

$$\overline{u_i u_j u_k} = -c_s' \frac{k}{\varepsilon} (\overline{u_i u_l} (\overline{u_j u_k})_{,l} + \overline{u_j u_l} (\overline{u_k u_i})_{,l} + \overline{u_k u_l} (\overline{u_i u_j})_{,l}) \quad (3.23)$$

To arrive at this term, Hanjalic and Launder assumed that: (i) the Reynolds number is large, (ii) the convection of $\overline{u_i u_j u_k}$ can be neglected, (iii) terms of the form

*This seems to be the only suggestion for modelling this term explicitly.

$\overline{u_i u_k u_l} \overline{u_i u_l}$ are much smaller than the gradients of the fourth order correlation $(\overline{u_i u_j u_k u_l})_{,1}$, (iv) the pressure-stress correlation is represented by:

$$\{\overline{u_i u_k p}_{,k} + \overline{u_j u_k p}_{,i} + \overline{u_k u_i p}_{,j}\} \propto \frac{\varepsilon}{k} \overline{u_i u_j u_k}$$

It was also assumed that the triple correlations are small and their distribution properties are sufficiently closely Gaussian for the Millionshtchikov (1941) formula* (exact for a Gaussian distribution) to apply:

$$\overline{u_i u_j u_k u_l} = \overline{u_i u_j} \overline{u_k u_l} + \overline{u_i u_k} \overline{u_j u_l} + \overline{u_i u_l} \overline{u_j u_k} \quad (3.24)$$

It is interesting to note that Donaldson's model for $\overline{u_i u_j u_k}$ can be retrieved from Hanjalic and Launder's equation (3.23) if $\overline{u_m u_l}$ (where $m = i, j$ or k) is set equal to $\frac{2k\delta}{3} \delta_{ml}$. i.e. by assuming isotropic diffusion coefficients.

A simpler model from (3.22) and (3.23) was given by Daly and Harlow (1970), as follows.

$$-\overline{u_i u_j u_k} = c_s \frac{k}{\varepsilon} \overline{u_k u_l} (\overline{u_i u_j})_{,l} \quad (3.25)$$

where c_s is a constant. Although equation (3.25) is not compatible as far as symmetry is concerned (for unlike the

*It should be stated that Andere et al (1976) have pointed out that from previous experience equation (3.24) when applied to a third order closure could lead to physically unrealistic results (see also Hinze (1975)).

left hand side, the right hand side alters under permutation of i, j and k); Launder et al (1975) however have reported that equation (3.25) exhibited satisfactory performance in predicting free shear flows; also Reece (1977) found, from predictions made for plane wall flows, that equation (3.25) performs almost equally as well* as the more numerically complicated form (3.23). Consequently Daly's and Harlow's simpler form (3.25) is employed in the present investigation. The value of c_s used was 0.25 which was obtained by Launder et al (1975) from computer optimisation.

(c) Pressure strain term: Following Chou (1945) an equation for the pressure fluctuation can be derived by taking the divergence of equation (3.3) and by applying the continuity constraint (2.15) to yield the following equation for $p^\pm$

$$\begin{aligned} -\frac{1}{\rho} p_{,nn} = & \bar{U}_{1,m} u_{n,1} + u_{1,n} u_{n,1} - \overline{u_{1,n} u_{n,1}} - \beta_n \theta_{,n} \\ & - \alpha_{nk} u_{k,n} \end{aligned} \quad (3.26)$$

The general solution of this equation consists of volume and surface integrals. Chou (1945) pointed out that the latter can be neglected in regions away from solid boundaries and hence the solution reduces to (Chou (1945)):

$$\begin{aligned} \frac{1}{\rho} p = & \frac{1}{2\pi} \int_{vol} \bar{U}'_{1,n} u'_{n,1} \frac{dV'}{|\underline{r}|} + \frac{1}{4\pi} \int_{vol} (u'_{1,n} u'_{n,1} - \overline{u'_{1,n} u'_{n,1}}) \frac{dV'}{|\underline{r}|} \\ & - \frac{\beta_n}{4\pi} \int_{vol} \theta'_{,n} \frac{dV'}{|\underline{r}|} - \frac{\alpha_{nk}}{4\pi} \int_{vol} u'_{k,n} \frac{dV'}{|\underline{r}|} \end{aligned} \quad (3.27)$$

*In a more recent publication Cormack et al (1978) reported that, from predictions made (wall jet, asymmetric channel, pipe flow and mixing layer), Daly and Harlow's model (3.25) displayed poorer results than Hanjalic and Launder's model.

‡The subscripts i and j are exchanged for n and 1 respectively.

where integration is carried over the whole region of the moving fluid; the x'_i ($i = 1, 2, 3$) are the coordinates of a point M' which ranges over the whole volume considered, $|\underline{r}|$ is the distance from M' to point M (at which the value of p is being calculated) with coordinates x_i and dV' is a volume element. Multiplying equation (3.27) by $u_{i,j}$ (at location M), and averaging and noting that by continuity $u_{1,n}u_{n,1} = (u_1u_n)_{,n1}$ yields the following equation for the pressure-strain correlation ϕ_{ij} :

$$\begin{aligned} \phi_{ij} = \frac{1}{\rho} \overline{pu_{i,j}} &= \frac{1}{4\pi} \int_{vol} \overline{(u_1u_n)_{,1n}u_{i,j}} \frac{dV'}{|\underline{r}|} + \frac{1}{2\pi} \int_{vol} \overline{\bar{u}'_{1,n}u_{i,j}u'_{n,1}} \frac{dV'}{|\underline{r}|} \\ &+ \beta_n \frac{1}{4\pi} \int \overline{\phi'_{,n}u_{i,j}} \frac{dV'}{|\underline{r}|} - \frac{\alpha_{nk}}{4\pi} \int \overline{u'_{k,n}u_{i,j}} \frac{dV'}{|\underline{r}|} \end{aligned} \quad (3.28)$$

$\phi_{ij,1}$ is the contribution to ϕ_{ij} due to the inertial interaction between turbulent velocities; Rotta (1951) noted that this term acts as an agent that reduces anisotropy of the flow. Thus if turbulence is left to its own dynamics in the absence of mean strain (and other influences), it would always tend to the isotropic state, for which $\phi_{ij,1}$ is then zero. From a purely physical argument Rotta (1951) (see also Hinze (1975)) suggested that $\phi_{ij,1}$ be approximated by:

$$\phi_{ij,1} = \frac{-2c_1k}{t_h} a_{ij} \quad (3.29)$$

where a_{ij} is the departure from isotropy tensor:

$$a_{ij} = \frac{\overline{u_i u_j}}{2k} - \frac{\delta_{ij}}{3}$$

t_h is the relaxation time of turbulence and c_1 is a constant. Originally Rotta identified the relaxation time as the decay time of isotropic turbulence k/ϵ ; Zeman (1975) however argued that experimental evidence suggests that turbulence returns faster to isotropy than it decays and furthermore the relaxation time must also be influenced by the input time scale k/P_T where P_T is the total production of k defined as

$$P_T = -\overline{u_i u_j} \overline{U_{i,j}} + \beta_i \overline{u_i \theta} \quad (3.30)$$

According to Zeman the relaxation time t_h should then be

$$t_h = k/(a\epsilon + bP_T) \quad (3.31)$$

where a and b are some constants. It should be noted that this time scale will be proportional to the one proposed by Rotta for self preserving flows. For the sake of simplicity Rotta's original proposal is retained here, hence:

$$(\phi_{ji} + \phi_{ij})_{,1} = -2c_1 \epsilon (a_{ji} + a_{ij}) \quad (3.32)$$

It should be mentioned that Lumley's procedure, outlined earlier, yields a similar expression if the series

he describes is truncated early and only linear terms in the non-isotropy tensor a_{ij} , are allowed (i.e. small non-isotropy is assumed).

Next $\phi_{ij,2}$ and $\phi_{ij,4}$ are considered; the first term is that part of ϕ_{ij} resulting from the interaction of turbulence with the mean strain rate and the second is due to the interaction of the Coriolis component of acceleration with turbulence. $\phi_{ij,2}$ and $\phi_{ij,4}$ are sometimes referred to as the 'rapid part of the pressure-strain correlation'.

In his analysis Chou (1945) suggested that the mean strain rate appearing in $\phi_{ij,2}$ can be expanded in a Taylor series about the point x_i and to simplify the mathematics involved he neglected* higher order terms. Following this practice the sum of $\phi_{ij,2}$ and $\phi_{ij,4}$ can then be written as:

$$\phi_{ij,2} + \phi_{ij,4} = (\bar{U}_{1,m} - \frac{\alpha_{1n}}{2}) a_{jl}^{in} \quad (3.33)$$

where

$$a_{jl}^{in} = \frac{1}{2\pi} \int (\overline{u_i u_n'})_{,jl} \frac{dv'}{|r|} \quad (3.34)$$

Defining ζ_i as

$$\zeta_i = x_i' - x_i \quad (3.35)$$

*This is consistent with mixing length assumptions.

then if a homogeneous turbulence is assumed then (see von-Karman and Haworth (1938))

$$\frac{\partial}{\partial \zeta_i} = \frac{\partial}{\partial x'_i} \equiv - \frac{\partial}{\partial x_i} \quad (3.36)$$

hence

$$a_{jl}^{in} = - \frac{1}{2\pi} \int_{vol} \frac{\partial^2 \overline{u_i u_n} dv' / |r|}{\partial \zeta_l \partial \zeta_j} \quad (3.37)$$

From (3.37) it can be noted that:

$$a_{jl}^{in} = a_{jl}^{ni} = a_{lj}^{in} = a_{lj}^{ni} \quad (3.38)$$

and by continuity:

$$a_{il}^{in} = a_{ji}^{in} = a_{nj}^{in} = a_{jn}^{in} = 0 \quad (3.39)$$

also it can be shown by carrying out the integral (3.37) (see Appendix C2) that

$$a_{jj}^{in} = 2 \overline{u_n u_i} \quad (3.40)$$

which was already obtained by Rotta (1951).

Equation (3.37) for the fourth order tensor a_{ln}^{ij} can be expressed as:

$$a_{lj}^{in} = F_{inlj}(\overline{u_k u_s}) \quad (3.41)$$

where F_{inlj} is a fourth-rank tensor functional of the value of the argument* taken over all values of x_i . For the condition of weak inhomogeneity assumed then the value of the argument can be taken as local. By using invariant theory (c.f. Lumley (1970)) the following relation for a_{lj}^{in} (see Appendix C3) is arrived at

$$\begin{aligned} a_{lj}^{in} = & a\delta_{lj}\delta_{ni} + b\overline{u_j u_l}\delta_{ni} + c\overline{u_k u_j}\overline{u_l u_n}\delta_{ni} + d\delta_{il}\delta_{nj} \\ & + e\overline{u_i u_l}\delta_{nj} + f\overline{u_i u_k}\overline{u_k u_l}\delta_{nj} + g\delta_{nl}\delta_{ji} + h\overline{u_n u_l}\delta_{ji} \\ & + i\overline{u_n u_k}\overline{u_k u_l}\delta_{ji} + j\delta_{nj}\delta_{il} + s\overline{u_n u_j}\delta_{il} + l\overline{u_n u_k}\overline{u_k u_j}\delta_{li} \\ & + m\delta_{ij}\delta_{ln} + n\overline{u_i u_j}\delta_{ln} + o\overline{u_i u_k}\overline{u_k u_j}\delta_{ln} + p\delta_{in}\delta_{lj} \\ & + q\overline{u_i u_n}\delta_{lj} + v\overline{u_i u_k}\overline{u_k u_n}\delta_{lj} \end{aligned} \quad (3.42)$$

where the coefficients $a, b, c \dots$ etc. are here functions of the invariants of the Reynolds stress. Applying the kinematic constraint (3.38) to (3.41) (details are given in Appendix C3) and then multiplying by the mean strain rate $\overline{U}_{n,l}$ and adding the result to the term $\overline{U}_{n,l}a_{li}^{jn}$ gives the following relation previously presented by Launder et al (1975):

$$\begin{aligned} (\phi_{ij} + \phi_{ji})^{\frac{\pi}{2}} = & -\frac{(c_1^1 + 8)}{11}\{P_{ij} - \frac{2P\delta_{ij}}{3}\} - \frac{(30c_1^1 - 2)}{55}k\{\overline{U}_{i,j} + \overline{U}_{j,i}\} \\ & - \frac{(8c_1^1 - 2)}{11}\{D_{ij} - \frac{2P\delta_{ij}}{3}\} \end{aligned} \quad (3.43)$$

*For non-homogeneous turbulence F_{inlj} is probably a functional of other quantities in addition to $\overline{u_k u_s}$.

$\frac{\pi}{2}\phi_{ij} \sim \phi_{ij}^4$ since $\phi_{ij}^4 / \phi_{ij}^2 \sim 1/Ro_1$.

where $P_{ij} = - \{ \overline{u_i u_k} \overline{U_{j,k}} + \overline{u_i u_k} \overline{U_{i,k}} \}$, $D_{ij} = - \{ \overline{u_i u_k} \overline{U_{k,j}} + \overline{u_j u_k} \overline{U_{k,i}} \}$ and c_2' is an undetermined constant.

It is interesting to note that for isotropic turbulence which is subjected to a sudden mean strain equation (3.43) reduces to the exact solution derived by Crow (1968)

$$(\phi_{ij} + \phi_{ji})_2 = 0.4k(\overline{U_{i,j}} + \overline{U_{j,i}}) \quad (3.44)$$

In Launder, Reece and Rodi (1975) it was proposed that a degenerate form for $(\phi_{ij} + \phi_{ji})$ such as*

$$(\phi_{ij} + \phi_{ji})_2 = - c_2(P_{ij} - \frac{2P\delta_{ij}}{3}) \quad (3.45)$$

could imitate the behaviour of $(\phi_{ij} + \phi_{ji})_2$ given by equation (3.44); this proposal was assessed by Launder et al (1975) for several test cases and it was found that the simpler version produced similar, albeit slightly inferior, quantitative results. In view of its much simpler form equation (3.45) is employed here.

The value of c_2 used is 0.6 in order to agree with Crow's result (3.44) for isotropic turbulence. With this value of c_2 , c_1 should be about 1.8 to satisfy the isothermal, homogeneous shear flow results of Champagne et al (1970).

The gravitational part of the pressure strain correlation, $\phi_{ij} \text{ }_3$, can be written for homogeneous turbulence as

*This relation was originally suggested by Naot et al (1973) though they employed it without including $\phi_{ij} \text{ }_1$.

$$\phi_{ij} = -\beta_n a_{nj}^i \quad (3.46)$$

where

$$a_{nj}^i = - \frac{1}{4\pi} \int_{vol} \frac{\partial}{\partial \zeta_n} \frac{\partial}{\partial \zeta_j} \overline{\theta u_i'} \frac{dV'}{|r|} \quad (3.47)$$

From symmetry and continuity a_{nj}^i satisfies respectively the relations

$$a_{nj}^i = a_{jn}^i \quad (3.48)$$

$$a_{ni}^i = a_{ij}^i = 0 \quad (3.49)$$

Further by carrying out the integration in (3.47)

$$a_{jj}^i = \overline{u_i \theta} \quad (3.50)$$

a_{nj}^i can in general be expressed as

$$a_{nj}^i = G_{inj}(\overline{u_k \theta}) \quad (3.51)$$

where G_{inj} is a third order tensor functional of the argument. With the assumption of weak inhomogeneity a_{nj}^i can be written as

$$a_{nj}^i = d \overline{u_i \theta} \overline{u_j \theta} \overline{u_n \theta} + a \overline{u_n \theta} \delta_{ji} + b \overline{u_j \theta} \delta_{in} + c \overline{u_i \theta} \delta_{jn} \quad (3.52)$$

where here a , b , c and d are functions of the invariants of $\overline{u_i \theta}$. Retaining only linear terms and applying the constraints (3.48) to (3.50), (3.52) yields (see appendix C3):

$$a_{nj}^i = 0.4 \overline{u_i \theta} \delta_{jn} - 0.1 (\overline{u_n \theta} \delta_{ji} + \overline{u_j \theta} \delta_{in}) \quad (3.53)$$

therefore*

$$(\phi_{ij} + \phi_{ji})_3 = -c_3 (G_{ij} - \frac{2}{3} \delta_{ij} G) \quad (3.54)$$

where G_{ij} and G are respectively the production rates of $\overline{u_i u_j}$ and k by buoyancy:

$$G_{ij} \equiv \beta_j \overline{u_i \theta} + \beta_i \overline{u_j \theta}$$

$$G \equiv \beta_i \overline{u_i \theta}$$

and c_3 is a constant equal (from (3.53)) to 0.3. Gibson and Launder (1978), however, found that a value of $c_3 = 0.5$ gave better results for wall-affected turbulence and hence their recommended value of c_3 (= 0.5) is employed here.

(d) Wall effects on the pressure-strain term: In the analysis of the pressure strain correlation the assumptions of weak non-homogeneity and non-isotropy were made; the formulae obtained are therefore not expected to perform well in

*This equation was given earlier by Launder (1975) and Lumley (1975).

regions far removed from the isotropic state, such as, for example, in near-wall flows. For this reason, and probably more importantly also because the surface integral in the solution of the Poisson equation for pressure (equation (3.27)) was neglected, it is necessary that some type of wall correction must be incorporated.

In devising a correction term for wall effects, the following restraints should be complied with:

- (i) The effect of the wall should diminish with distance from it.
- (ii) The corrective term must have the same tensor characteristics as $\overline{p_{i,j}}$ and must moreover be tensor invariant.
- (iii) The term should reproduce the important characteristics of experimental observations.

Shir (1973) developed a model to describe wall effects which was originally proposed by Daly and Harlow (1970).

Shir's suggestion can be written as

$$\phi_{ij1w} = c'_1 \frac{\varepsilon}{k} (\overline{u_k u_m} n_k n_m \delta_{ij} - \frac{3}{2} \overline{u_i u_k} n_k n_j - \frac{3}{2} \overline{u_j u_k} n_k n_i) f\left(\frac{1}{n_i r_i}\right) \quad (3.55)$$

where c'_1 is a constant, n_i is the unit vector normal to the ground and r_i is the position vector.

Shir's proposal does not allow for wall influences on $\phi_{ij,2}$ or $\phi_{ij,3}$; recognising this deficiency, Gibson and Launder (1978) extended Shir's formulation to include a mean strain contribution $\phi_{ij,2w}$ and a gravitational one $\phi_{ij,3w}$. Their proposals are:

$$\phi_{ij \ 2w} = c'_2 \left(\phi_{km} \ 2^n_k n_m \delta_{ij} - \frac{3}{2} \phi_{ki} \ 2^n_k n_j - \frac{3}{2} \phi_{kj} \ 2^n_k n_i \right) f\left(\frac{1}{n_i r_i}\right) \quad (3.56)$$

$$\phi_{ij \ 3w} = c'_3 \left(\phi_{km} \ 3^n_k n_m \delta_{ij} - \frac{3}{2} \phi_{ki} \ 3^n_k n_j - \frac{3}{2} \phi_{jk} \ 3^n_k n_i \right) f\left(\frac{1}{n_i r_i}\right) \quad (3.57)$$

where c'_2 and c'_3 are constants.

The effects of $\phi_{ij \ 2w}$ and $\phi_{ij \ 3w}$ are similar to that of $\phi_{ij \ 1w}$ in that they enhance anisotropy by draining energy from the normal component of the Reynolds stress and distributing it equally between the tangential components. Experimental data reveal that the effect of the wall is indeed to transform energy from the normal to the tangential components; however, unlike (3.55) to (3.57) suggest, the measurements show that the longitudinal fluctuations receive most of the energy transformed.

In a comparison, by Samaraweera (1978), between the performances of the Gibson and Launder (1978) wall-correction model and an earlier one given by Launder et al (1975), it was found that while the latter performs better in predicting the non-dimensionalised (by the wall shear stress) longitudinal and lateral turbulent stresses of Klebanoff's (1954) experiment the two models gave similar results for the vertical and shear turbulent stresses. Samaraweera (1978) also reported that the Gibson and Launder (1978) model gave better prediction for the wall shear stress; consequently it was found that in absolute (dimensional) terms the two models performed equally well.

The attractiveness of the Gibson and Launder (1978) near-wall correction is that its extension to the case of the pressure-scalar gradient is obvious; accordingly it is applied in the present analysis.

The values of c_1' and c_2' employed were obtained by Gibson and Launder (1978) by appeal to near wall flows; these were 0.5 and 0.3 respectively. c_3' appears to have little influence on predictions of stratified wall flows (close to the wall buoyancy effects are usually small; see for example Monin and Yaglom (1977)) and it was consequently set to zero.

The function $f(\frac{1}{r_i n_i})$ acts as a mechanism that reduces the wall effect as the distances from it increase. Samaraweera (1978) has examined the performance of two such functions. The first, proposed by Launder et al (1975), was:

$$f\left(\frac{1}{r_i n_i}\right) = \frac{k^{3/2}}{a \epsilon x_3} \quad (3.58)$$

where a is a constant. The second function was suggested by Gibson and Launder (1978) this has the form:

$$f\left(\frac{1}{r_i n_i}\right) = \frac{(-\overline{u_1 u_3})^{3/2}}{a'' \epsilon x_3} \quad (3.59)$$

where a'' is a constant.

From comparisons made with Klebonoff's (1954) flat plate boundary layer experimental data, Samaraweera concluded that equation (3.58) was superior to the function given by

(3.59). Accordingly (3.58) is employed here. The value of constant a was set equal to 3.28 so as to give a value of unity for $f\left(\frac{1}{r_1 n_1}\right)$ close to the wall.

Modelled equation of $\overline{u_i u_j}$ and k - Assembling the various selected proposals leads to the following modelled transport equation for $\overline{u_i u_j}$:

$$\begin{aligned} \overline{u_k} (\overline{u_i u_j})_{,k} = & - (\overline{u_i u_k} \overline{u_j}_{,k} + \overline{u_j u_k} \overline{u_i}_{,k}) + (\beta_i \overline{\theta u_j} + \beta_j \overline{\theta u_i}) \\ & - \frac{1}{3} \epsilon \delta_{ij} - c_s \frac{k}{\epsilon} \overline{u_k u_l} (\overline{u_i u_j})_{,l},_{k} + (\phi_{ij} + \phi_{ji})_1 + (\phi_{ij} + \phi_{ji})_2 \\ & + (\phi_{ij} + \phi_{ji})_3 + (\phi_{ij} + \phi_{ji})_{1w} + (\phi_{ij} + \phi_{ji})_{2w} + (\phi_{ij} + \phi_{ji})_{3w} \end{aligned} \quad (3.60)$$

where the ϕ_{ij} 's are given by relation (3.32), (3.45), (3.54), (3.55), (3.56) and (3.57) respectively.

By taking the trace of equation (3.60) we obtain the following modelled equation for k :

$$\overline{u_i k}_{,i} = - \overline{u_i u_k} \overline{u_i}_{,k} + \beta_i \overline{\theta u_i} - \epsilon + c_s \frac{k}{\epsilon} \overline{u_k u_l k}_{,l},_{k} \quad (3.61)$$

The values of the constants employed are summarised in Table 3.1.

3.3.2 Dissipation equation

The dissipation rate ϵ plays a very significant role in the present model, unfortunately it is the least tractable of all the turbulence equations considered. In particular the lack of measurements for any of the unknown terms on the

right hand side of equation (3.15) has prevented attempts of correlating these to other known variables and hence most of the efforts made to close the equation are basically intuitive.

(a) Production and dissipation term: Experimental evidence reveals that in isotropic turbulence the time scale of the decay of kinetic energy is of the order of the characteristic time of the energy containing eddies (Batchelor (1959)) thus:

$$\frac{Dk}{Dt} = \epsilon = - bu'^3/l \quad (3.62)$$

where D/Dt is the total derivative and b is some constant of order unity. As there are no macroscopic* time scales other than $k/\epsilon (\sim u'/l)$ it is reasonable to assume that in isotropic turbulence the dissipation rate decays with the same time scale as k , thus

$$\frac{D^2k}{Dt^2} = \frac{D\epsilon}{Dt} = - c_{\epsilon 2} \frac{\epsilon^2}{k} \quad (3.63)$$

where $c_{\epsilon 2}$ is a constant. Comte-Bellot and Corrsin (1966) found from their grid generated turbulence measurements that

*In equilibrium flows at high Re_l the dissipation rate, which has its main energy contribution from the high frequency eddies, is equal to the spectral energy flux. The former has a response time of the order u'/λ while the latter, which is dictated by the large scale motion, has a time scale proportional to u'/l . Now, since the governing mechanism of dissipation is the spectral transfer (in other words it is spectral transfer that decides how much energy is to be dissipated and not the viscosity) the dissipation rate is governed by the large scale motion (c.f. Tennekes and Lumley (1974)).

in isotropic turbulence k decays as x_1^{-n} where n is approximately 1.2; from equations (3.62) and (3.63) it can be shown that corresponding value of $c_{\epsilon 2}$ would then be about 1.9.

It is important to note that while the nature of the right hand side term is dissipative it must not be implied that this term is equal to the dissipation term in (3.15) but rather as the difference between the dissipation and production rates of ϵ (as argued by Von-Karman and Howarth (1938), the production term of ϵ is not necessarily zero in isotropic turbulence).

In the presence of a mechanical production term P of turbulence kinetic energy, the rate of spectral energy transfer (neglecting turbulent diffusion for the moment) will increase due to the accompanying increase in the turbulence. This will in turn influence the dissipation rate ϵ (c.f. Tennekes and Lumley). Several workers (e.g. Jones and Launder (1972)) have suggested the following form for the dissipation equation to account for the existence of the production* P :

$$\bar{U}_j \epsilon_{,j} = \left(\frac{c_{\epsilon 1} P}{c_{\epsilon 2}} - \epsilon \right) c_{\epsilon 2} \frac{\epsilon}{k} \quad (3.64)$$

where $c_{\epsilon 1}$ is a constant.

Lumely and Khajeh-Nouri (1974) use $a_{ij} a_{ji} \epsilon$ instead of P in equation (3.64), arguing that the spectral flux is affected

*Neglecting for the moment diffusion of ϵ .

by anisotropy of the turbulence components, and thus even in the absence of mean strain if the flow is non-isotropic generation of ϵ will still exist. At any rate in equilibrium flows the two terms (i.e. $a_{ij}a_{ji}\epsilon$ and P) are proportional and the two closures become similar.

For stratified flows Gibson and Launder (1976) argue that because the buoyant term $2\nu\beta_i\overline{\theta_{,1}u_{i,1}}$ in the dissipation equation (3.8) vanishes for large Reynolds number then no buoyancy term should explicitly appear in the transport equation for ϵ . However buoyancy effects do change the shape of the energy spectrum (Kaimal et al (1972), Panofsky and Deland (1959)) and should therefore in turn affect the energy cascade process. Thus allowance for buoyancy production is necessary for the same reason that mechanical production P is included. The most obvious extension of equation (3.64) to account for buoyancy effects is to replace P by P_ϵ defined as

$$P_\epsilon = P + \frac{c'_{3\epsilon}}{c_{\epsilon 1}} \overline{u_i \theta \beta_i} \quad (3.65)$$

where $c'_{3\epsilon}$ is a constant. This form was previously adopted by Svensson (1978) and Ideriah (1977), though they proposed the term as a modelled representation of $2\nu\beta_i\overline{\theta_{,1}u_{i,1}}$, which was argued earlier to be small at large Reynolds numbers.

In the present study the modelled form (3.64) of P_ϵ was found to work reasonably well in unstable stratified flows at small flux Richardson numbers, but as the latter was increased it was observed that ϵ increased drastically

which caused a reduction in k (the increase in ϵ overshadowed the increase in buoyancy production of k). It was therefore necessary to find a means of restraining ϵ from excessive increase at large Richardson numbers.

The following multiplying function F_ϵ when inserted in (3.65) gave the required effect (i.e. reduction of the buoyant term at large $\bar{u}_3^2/k$).

$$F_\epsilon = n_j \frac{u'_j}{\bar{u}_j} \quad (3.66)$$

where $u'_j = \sqrt{\bar{u}_j^2}$. The basis for choosing (3.66) was that F_ϵ should be a scalar, dimensionless and further must diminish the buoyancy term with increase in the Richardson number. When the term F_ϵ is included in equation (3.65), the latter becomes

$$P_\epsilon = P + \frac{c_{3\epsilon} \beta_i \bar{u}_i \bar{\theta} n_j}{c_{1\epsilon}} \frac{u'_j}{\bar{u}_j} \quad (3.67)$$

(b) Diffusion term: By severely truncating the transport equation for the diffusion term $\overline{v u_{i,1} u_{i,1}}$ Hanjalic and Launder (1972b) proposed the following model to represent the diffusion of ϵ by turbulent motion in boundary layer flows

$$(\overline{v u_{i,1} u_{i,1}})_{,k} = - c_{\frac{k}{\epsilon}} \frac{\overline{u_{i,1} u_{i,1}}}{\epsilon} \epsilon_{,k} \quad (3.68)$$

This is effectively an eddy diffusivity model with an equi-

valent effective diffusion coefficient for two-dimensional boundary layer flow given by:

$$K_{\epsilon} = c_{\epsilon} \frac{k}{\epsilon} \overline{u_3^2}$$

In a similar approach based on the transport equation of the turbulent diffusion term of ϵ in buoyant flows Zeman and Lumley (1976) arrived at a similar form to (3.68) but with an implied diffusivity that depends on the amount of stratification, thus

$$K_{\epsilon} = c_{\epsilon} \frac{k}{\epsilon} (\overline{u_3^2} + 0.31\beta_3 t'_{\theta} \overline{u_3 \theta}) \quad (3.69)$$

where t'_{θ} is the thermal time scale $\overline{\theta^2}/\epsilon_{\theta}$.

Equation (3.69) differs from that of Hanjalic and Launder by a buoyant term $0.31\beta_3 t'_{\theta} \overline{u_3 \theta}$; the effect of the latter is to increase K_{ϵ} in unstable flows while reducing it in stable flows.

A more complicated modelled form for the diffusion of ϵ term is given by Zeman (1975) who suggested that diffusion of ϵ in buoyant flows is achieved not only by gradients in ϵ but also by heat-flux gradients.

Though there are indications that buoyancy effects seem to affect explicitly the diffusion of ϵ , neither Lumley and Zeman's (1976) nor Zeman's (1975) suggestions have been properly tested here and Hanjalic and Launder's (1972b) proposal was the one employed.

Modelled dissipation equation: Insertion of relations

(3.64), (3.65) and (3.68) in equation (3.15) leads to the following proposed dissipation equation:

$$\frac{D\varepsilon}{Dt} = c_{\varepsilon 1} \frac{\varepsilon}{k} (P + \frac{c_{\varepsilon 3} \beta_i \overline{u_i \theta} n_j \overline{u_j'}}{c_{\varepsilon 1}}) - c_{\varepsilon 2} \frac{\varepsilon^2}{k} + c_{\varepsilon} (\frac{k \overline{u_i u_i}}{\varepsilon} \overline{u_i \varepsilon_i})_{,k} \quad (3.70)$$

A relation between the constants $c_{\varepsilon 1}$, $c_{\varepsilon 2}$ and c_{ε} is obtained by appeal to neutral near-wall flows, where the production and dissipation rates of k are approximately equal. By neglecting the convection term, equation (3.70) reduces in these circumstances to the algebraic relation

$$c_{\varepsilon} = \frac{(c_{\varepsilon 2} - c_{\varepsilon 1}) u_*^6}{\kappa^2 k^2 \overline{u_3^2}} \quad (3.71)$$

Since there are no further simple constraining equations c_{ε} and $c_{\varepsilon 1}$ must be obtained by reference to measurements of more complex flows and computer optimisation. Launder et al (1975) arrived in this fashion at $c_{\varepsilon 1} = 1.44$, and hence $c_{\varepsilon} = 0.17$.

In the present analysis the value of $c_{\varepsilon 3}$ was found by trial and error to be about 1.55. This was chosen so as to give the closest agreement between the predicted dimensionless velocity gradient (in the atmospheric boundary layer) $\phi_m (\equiv \overline{U}_{1,3} \kappa x_3 / u_*)$, and the modified KEYPS Formula (Businger et al (1971))

$$\phi_m = (1 - b_2 \frac{x_3}{L})^{0.25} \quad (3.72)$$

where L is the Monin-Obukhov length scale defined in equation (4.49) and b_2 is a constant.

3.3.3 Turbulent heat flux equation

As mentioned earlier, terms that require to be modelled in the transport equation of $\overline{u_i \theta}$ are the gravitational,

pressure-temperature gradient and the diffusion terms.

Special considerations apply to the latter which are discussed elsewhere in section 3.4; which leaves the gravitational and pressure temperature gradient to be modelled here.

(a) Gravitational term: In a second order closure the most consistant approach of calculating $\bar{\theta}^2$ is by way of solving an approximated transport equation similar to that of k . However because $\bar{\theta}^2$ plays a less dominant role in the model equations than k ; in the interest of economy the equation for $\bar{\theta}^2$ is transformed, under certain assumptions to an algebraic equation.

If it is assumed that the ratio R_θ of the time scales of the scalar field and the hydrodynamic field written as:

$$R_\theta = \bar{\theta}^2 / \epsilon_\theta / 2k / \epsilon \quad (3.73)$$

is constant and if it is moreover assumed that the production of $\bar{\theta}^2$ and its dissipation rate are equal i.e. if the transport term in the equation of $\bar{\theta}^2$ are negligible (c.f. Launder (1974)) then:

$$\bar{\theta}^2 = - \frac{k c_\theta}{\epsilon} \overline{u_j \theta} \bar{\theta}_{,j} \quad (3.74)$$

and hence the gravitational term becomes

$$\beta_i \bar{\theta}^2 = - \frac{k \beta_i c_\theta}{\epsilon} \overline{u_j \theta} \bar{\theta}_{,j} \quad (3.75)$$

where $c_\theta = 2R_\theta$. The value of R_θ reported in the literature

vary from 0.5 - 0.8 (c.f. Launder (1976)). Here the value of $R_\theta = 0.8$ suggested by Gibson and Launder (1978) is employed.

(b) Pressure-temperature gradient term: This term is the counterpart in the heat flux equation to the pressure-strain correlation in the Reynolds stress equation. It is normally the only mechanism, in neutral flows, that acts to diminish $\overline{u_i \theta}$.

The exact equation for the $\overline{u_i \theta}$ correlation is obtained by multiplying equation (3.27) for $\overline{p}$ by $\theta_{,i}$, and then time averaging the product. The following result is then obtained:

$$\begin{aligned} \overline{\frac{p\theta}{\rho}}_{,i} &= \frac{1}{4\pi} \int_{vol} \overline{(u_l u_n)'_{,ln} \theta_{,i}} \frac{dV'}{|\underline{r}|} + \frac{1}{2\pi} \int_{vol} \overline{\bar{u}'_{i,n} \bar{u}'_{n,l} \theta_{,i}} \frac{dV'}{|\underline{r}|} \\ &\quad - \frac{\beta_i}{4\pi} \int_{vol} \overline{\theta'_{,n} \theta_{,i}} \frac{dV'}{|\underline{r}|} - \frac{\alpha_{nk}}{4\pi} \int_{vol} \overline{u'_{k,n} \theta_{,i}} \frac{dV'}{|\underline{r}|} \end{aligned} \quad (3.76)$$

Here the term ϕ_{ic1} is of similar nature to ϕ_{ij1} in $\overline{u_i u_j}$ equation: Monin (1965) modelled this term in an analogous manner to Rotta's 'return to isotropy' term (3.29) i.e.

$$\phi_{ic1} = -c_{1c} \frac{\overline{u_i \theta}}{t_\theta} \quad (3.77)$$

where t_θ is a relaxation time of the turbulence field. This form has been used extensively by many authors e.g. Launder (1975), Donaldson (1972), Zeman (1975). A more complicated

model for $\phi_{ic,1}$ that included non-linear terms in $\overline{u_i c}$ was proposed by Lumley (1975).

Zeman (1975) assumed that the scalar field will return to isotropy within the same time scale as the hydrodynamic field and hence used equation (3.31) to calculate t_θ . Launder (1975) suggested that t_θ should reflect the time scales of both the scalar and hydrodynamic fields: however he argued that in equilibrium flows all time scales are proportional and he consequently used the hydrodynamic time scale k/ϵ .

It is consistent with the assumption of constant R_θ (which implies equilibrium) to take t_θ as proportional to the time scale k/ϵ : when this is done equation (3.77) becomes

$$\phi_{ic1} = -c_{1c} \frac{\epsilon}{k} \overline{u_i \theta} \quad (3.78)$$

By neglecting second derivatives of the velocity field the 'rapid' parts of ϕ_{ic} , ϕ_{ic2} and ϕ_{ic4} can be combined to yield

$$\phi_{ic2} + \phi_{ic4} = (\overline{U}_{1,n} - \frac{\alpha_{1n}}{2}) 2a_{1i}^n \quad (3.79)$$

where a_{1i}^n was defined earlier in equation (3.47). For homogeneous conditions

$$2a_{1i}^n = .8 \overline{u_n \theta} \delta_{1i} - .2 (\overline{u_1 \theta} \delta_{in} + \overline{u_i \theta} \delta_{1n}) \quad (3.80)$$

If α_{1n} is neglected in comparison to $\bar{U}_{1n}$, the rapid part reduces to

$$\phi_{ic2} = 0.8 \bar{u}_n \bar{\theta} \bar{U}_{i,n} - 0.2 \bar{u}_n \bar{\theta} \bar{U}_{n,i} \quad (3.81)$$

Lauder (1975) suggested a simpler form for ϕ_{ic2} that has the merit of yielding simpler algebraic results and has also been used extensively; the Lauder proposal is analogous to the form given by equation (3.45), i.e.

$$\phi_{ic2} = -c_{2c} \bar{u}_n \bar{\theta} \bar{U}_{i,n} \quad (3.82)$$

where c_{2c} is a constant. In the present investigation the simpler model (3.82) is employed. It is to be noted that in a two dimensional boundary layer ϕ_{2c2} and ϕ_{3c2} will be negligible.

Finally, the buoyancy term ϕ_{ic3} can be written as

$$\phi_{ic3} = -\beta_k a_{ik} \quad (3.83)$$

where

$$a_{ik} = -\frac{1}{4\pi} \int_{vol} \frac{\partial \theta' \partial \theta'}{\partial \zeta_i \partial \zeta_k} \frac{dV'}{|\underline{r}|} \quad (3.84)$$

It is shown in Appendix C1 that for isotropic turbulence

$$a_{ii} = \bar{\theta}^2 \quad (3.85)$$

Now a_{ik} can be expressed as a second rank tensor functional of $\bar{\theta}^2$ taken over all values of x_i . By assuming weak inhomogeneity the local value of $\bar{\theta}^2$ can be used, and hence the tensor invariant form of a_{ik} reads

$$a_{ik} = c_{3c} \bar{\theta}^2 \delta_{ik} \quad (3.86)$$

c_{3c} being a constant. With relation (3.86), equation (3.83) may be written as*

$$\phi_{ic3} = -c_{3c} \beta_i \bar{\theta}^2 \quad (3.87)$$

Constraint (3.85) together with equation (3.86) yields a value of $c_{3c} = 1/3$.

(c) Wall effects on pressure-temperature gradient: For similar reasons to those discussed earlier in connection with the stress modelling a near wall correction should also be applied to ϕ_{ic} . Gibson and Launder (1978) extended their suggestion of ϕ_{ij1w} , ϕ_{ij2w} and ϕ_{ij3w} to the scalar field and proposed the following counterparts for the wall correction of the scalar field.

$$\phi_{ic1w} = c'_{ic} \frac{\epsilon u_k}{k} \bar{\theta} n_i n_k f\left(\frac{1}{n_i r_i}\right) \quad (3.88)$$

* $\bar{\theta}^2$ is obtained from equation (3.74).

$$\phi_{ic2w} = c'_{2c} c_{2c} P_{k\theta} n_i n_k f\left(\frac{1}{n_i r_i}\right) \quad (3.89)$$

$$\phi_{ic3w} = c'_{3c} c_{3c} G_{k\theta} n_i n_k f\left(\frac{1}{n_i r_i}\right) \quad (3.90)$$

where $P_{k\theta}$ and $G_{k\theta}$ are the production of $\overline{u_k \theta}$ by mean shear and buoyancy respectively i.e.

$$P_{i\theta} = -\overline{u_k \theta} \overline{U}_{i,k} \quad (3.91)$$

$$G_{i\theta} = \beta_i \overline{\theta}^2 \quad (3.92)$$

and c'_{1c} , c'_{2c} and c'_{3c} are constants.

The value of c'_{1c} is obtained by reference to near wall flows and this was found to be 0.5. In two dimensional flows $P_{3\theta}$ is small and hence the solution is independent of the value of c'_{2c} . c'_{3c} similar to c_{3w} is set to zero.

Modelled equation for turbulent heat flux: The proposed

modelled transport equation for $\overline{u_i \theta}$ finally has the form

$$\begin{aligned} \frac{D}{Dt} \overline{u_i \theta} = & -(\overline{u_i u_j} \overline{\theta}_{,j} + \overline{u_i \theta} \overline{U}_{i,j}) - \beta_i \frac{k c_{\theta}}{\epsilon} \overline{u_j \theta} \overline{\theta}_{,j} \\ & + \phi_{ic,1} + \phi_{ic,2} + \phi_{ic,3} + \phi_{ic1w} + \phi_{ic2w} + \phi_{ic3w} \\ & + \mathcal{Q}(\overline{u_i \theta}) \end{aligned} \quad (3.93)$$

where the operator $\mathcal{Q}(\)$ refers to diffusion of (...). The ϕ terms are defined by equation (3.78), (3.82), (3.87) and (3.88), (3.89) and (3.90). The constants appearing in these

are summarised in Table 3.1.

3.3.4 Turbulent species concentration flux equation

No major differences exist between the terms in the equations for $\overline{u_i c}$ and for $\overline{u_i \theta}$ and generally the same modelling is employed for both. However two particular differences arise here; the first is due to the fact that while θ is coupled to the flow field via buoyancy effects C is not. The second arises from the particular approach adopted in specifying the time scales*.

All terms in $\overline{u_i c}$ equation where the dissimilarities mentioned do not appear are modelled in a similar fashion to their counterparts in the $\overline{u_i \theta}$ equation and are not therefore considered below.

(a) Buoyancy term: The buoyancy term appearing in equation (3.19) contains the unknown correlation $\overline{c\theta}$ between the passive scalar c and the active one ϕ . In appendix C4 a modelled equation for $\overline{c\theta}$ is suggested; if the production rate of $\overline{c\theta}$ is assumed equal to the dissipation rate then according to the proposition given in appendix C4, $\overline{\theta c}$ can be obtained from the algebraic expression

$$\overline{c\theta} = -a' \frac{k}{\epsilon} (\overline{cu_j \theta},_j + \overline{u_j \theta C},_j) \quad (3.94)$$

where a' is a constant. It is set here equal to 0.9. This value for a' was chosen, as will be explained in chapter 6,

*Had equations for ϵ_θ , $\overline{\theta^2}$ and ϵ_c , $\overline{c^2}$ been solved no problems in specifying the time scales would have arisen.

so that predictions of the vertical pollutant dispersal in a stratified atmosphere^{were} to be in good agreement with experimental observations.

(b) Pressure concentration gradient: The equation for $\overline{pc}_{,i}$ is nearly identical to that for $\overline{p\theta}_{,i}$: the only differences will be in the form of $\phi_{ic,3}$ and in the specification of the time scale in $\phi_{ic,1}$, which need not be the same as those for $\overline{p\theta}_{,i}$.

It was stated previously that the time scales of the scalar and hydrodynamic fields are often assumed to be proportional. Although such an assumption is, in the situations considered here, valid for the temperature field, it is not expected to hold at the early stages of development of the plume concentration field as will be explained below.

An indicative value of the time scale of the turbulent motion is given by (Batchelor (1959)):

$$t_h = a_1 l' / u' \quad (3.95)$$

where a_1 is some constant. Correspondingly the time scale t_c of the fluctuations of the concentration can be estimated as:

$$t_c = a_2 l_c / u' \quad (3.96)$$

where a_2 is another constant and l_c is a length scale of the concentration field.

From (3.95) and (3.96) the time scale ratio between t_c and t_h , R_c is then:

$$R_c = \frac{t_c}{t_h} = \frac{a_1}{a_2} \frac{l_c}{l} \quad (3.97)$$

Now when the plume dimensions are much smaller than the length scale of the turbulent field as for example in the initial stages of dispersal of a plume from an elevated point source, the plume could be viewed as if it was in a homogeneous turbulence; and hence according to Taylor's equation (1.7) l_c (for small diffusion times) would increase as x_1 ; while l is approximately constant. Consequently R_c cannot be assumed constant i.e. t_c and t are not proportional. For large downstream (of the source) distances when the plume has grown such that l and l_c are of the same order of magnitude, the length scales could be expected to increase at the same rate and R_c is then constant. By contrast a plume emanating from a ground level source the sizes of eddies there are limited by their distance from the ground and consequently l and l_p could be proportional from the onset of the dispersal process.

It is interesting to note the consequences of employing equation (3.93) (using the hydrodynamic time scale t_h to predict the turbulent diffusion of a plume released from a point source into a homogeneous turbulent field. If the transport terms* are neglected then:

$$\overline{u_3 c} = - \frac{1}{c_{1c}} \overline{u_3^2 k C}_{,3} \quad (3.97)$$

which implies a diffusivity K_3

*This is a rough approximation.

$$K_3 = \frac{1}{c_{1c}} \frac{\overline{u}_3^2 k}{\epsilon} \quad (3.98)$$

Since the turbulent field is assumed to be homogeneous then from (3.98) K_3 is a constant independent of the diffusion time. This is in contradiction with the results of Taylor's equation (1.7) for short diffusion times.

The above drawback could be remedied by using the time scale of the concentration fluctuation $\overline{c}^2/\epsilon_c$ for t_c , but this would require knowledge of $\overline{c}^2$ and ϵ_c which for reasons mentioned are not calculated here. An alternative approach is to estimate t_c using mixing length concepts. Thus if l_c is taken as proportional to the width of the plume δ_c , then from equation (3.97)

$$R_c = \frac{t_c}{t_h} = a_3 \frac{\delta_c \epsilon}{k^{3/2}}$$

or

$$t_c = a_3 \frac{\delta_c}{k^{1/2}} \quad (3.100)$$

where a_3 is a constant.

By equating t_ϕ in the equation of ϕ_{ic1} with the above, there results

$$\phi_{ic1} = -c_{1c} \frac{a_3}{\delta_c} k^{1/2} \overline{u_i c} \quad (3.101)$$

The value of a_3 was found by trial and error to be 0.55. The criterion for the choice of a_3 was that the numerically predicted values of σ_2 to be in agreement with the results of the elevated point source experiments carried out in the present study.

The buoyancy term ϕ_{ic3} of the pressure, concentration gradient term, reads

$$\phi_{ic3} = \frac{-\beta_k}{4\pi} \int_{vol} \frac{\overline{\theta_k c}_{,i} dV'}{|\underline{r}|} \quad (3.102)$$

If a similar procedure is followed as with (3.87) the above can be written as

$$\phi_{ic3} = -\frac{1}{3} \beta_1 \overline{c\theta} \quad (3.103)$$

Modelled equation for concentration flux: By replacing θ and $\bar{\theta}$ by c and $\bar{C}$ respectively, collecting the buoyancy effected terms and using ϕ_{ic1} as defined by equation (3.101), the final modelled transport equation for $\overline{u_i c}$ then reads:

$$\begin{aligned} \frac{D}{Dt} \overline{u_i c} = & - (\overline{u_i u_j c}_{,j} + \overline{u_i c} \overline{u_{i,j}}) + \phi_{ic,1} + \phi_{ic,2} + \phi_{ic} w_1 \\ & + \phi_{ic} w_2 + \phi_{ic} w_3 + \overline{u_i c} - \frac{2a'k}{3\varepsilon} (\overline{cu_j \theta}_{,j} + \overline{u_j \theta C}_{,j}) \end{aligned} \quad (3.104)$$

3.4 Algebraic flux model

Though in principle it is possible to numerically solve the full modelled partial-differential equations for

the turbulent fluxes $\overline{u_i u_j}$, $\overline{u_i \theta}$ and $\overline{u_i c}$, it is worth while, in so far as computer time and storage requirements are concerned, to reduce these equations to a much simpler set of algebraic relations when circumstances allow.

Realising that it is the convection and diffusion transport terms which render the Reynolds stress equations strongly differential in character, Rodi (1972) proposed that by assuming the total transport of $\overline{u_i u_j}$ is proportional to the total transport of turbulence energy k , i.e.:

$$\begin{aligned} (\text{convection-diffusion})_{\text{of } \overline{u_i u_j}} &= \frac{\overline{u_i u_j}}{k} (\text{convection-diffusion})_{\text{of } k} \\ &= \frac{\overline{u_i u_j}}{k} (P_T - \epsilon) \quad (3.105) \end{aligned}$$

then the Reynolds stress equations are reduced to algebraic form.

The above assumption is valid when the characteristics of the turbulence as represented by the ratio $\overline{u_i u_j}/k$ vary but slightly relative to the variation of $\overline{u_i u_j}$ itself. Such an assumption is expected to hold in the self-preserving and weakly developing flows which are the main concern of the present investigation. However in certain circumstances, such as when large changes in surface roughness occur and give rise to strong non-equilibrium effects, the assumption undoubtedly gives rise to some error.

If the modelled Reynolds stress equation (3.61) is combined with equation (3.105), the transport equation for $\overline{u_i u_j}$

reduces to

$$\begin{aligned} \overline{u_i u_j} (P_T - \epsilon) = & P_{ij} + G_{ij} + (\phi_{ij} + \phi_{ji})_1 + (\phi_{ij} + \phi_{ji})_2 \\ & + (\phi_{ij} + \phi_{ji})_3 + (\phi_{ij} + \phi_{ji})_{1w} + (\phi_{ij} + \phi_{ji})_{2w} + (\phi_{ij} + \phi_{ji})_{3w} \end{aligned} \quad (3.106)$$

Laundier (1976) extended Rodi's ideas to the scalar flux equations; by assuming that the variation in $\overline{\phi u_i} / \sqrt{k} \sqrt{\overline{\phi^2}}$ (where ϕ here is used to denote either concentration or temperature) is less than that of either $\overline{\phi^2}$ or k ; this led to the proposal that:

$$\frac{D \overline{\phi u_i}}{Dt} - \overline{u_i \phi} = \overline{u_i \phi} \left(\frac{P_\phi - \epsilon_\phi}{2 \overline{\phi^2}} + \frac{P_T - \epsilon}{2k} \right) \quad (3.107)$$

where P_ϕ and ϵ_ϕ are the production and dissipation rates of $\overline{\phi^2}$. If it is further assumed* that P_ϕ and ϵ_ϕ are equal, then the transport equation for the turbulent scalar fluxes $\overline{u_i \phi}$ can be written as

$$\begin{aligned} \overline{u_i \phi} \frac{(P_T - \epsilon)}{2k} = & -(\overline{u_i u_j} \overline{\phi_{i,j}} + \overline{u_i \phi} \overline{u_{i,j}}) + G_{i\phi} + \phi_{ic1} + \phi_{ic2} \\ & + \phi_{ic3} + \phi_{ic1w} + \phi_{ic2w} + \phi_{ic3w} \end{aligned} \quad (3.108)$$

where ϕ is either c or θ and $G_{i\phi}$ is the buoyant production of $\overline{u_i \phi}$.

*Note that such an assumption could be quite crude when applied to the concentration fluctuation $\overline{c^2}$ in the immediate vicinity of the source; for as mentioned by Robins and Fackrell (1979) transport terms there could be significant.

3.5 Summary of the modelled equations

For the conditions assumed here i.e. three dimensional concentration field embedded in a two dimensional velocity and temperature field; the versions of the modelled equations employed in the present investigation reduce to the following relations.

3.5.1 Differential equations

(a) Turbulence kinetic energy

$$\bar{U}_1 k_{,1} + \bar{U}_3 k_{,3} = P + G + c_s \left(\frac{k \bar{u}_3^2}{\epsilon} \right)_{,3} - \epsilon \quad (3.109)$$

$$P = -\overline{u_1 u_3} \bar{U}_{1,3}, \quad G = \frac{g}{\theta_m} \bar{\theta} u_3$$

(b) Dissipation

$$\bar{U}_1 \epsilon_{,1} + \bar{U}_3 \epsilon_{,3} = c_{\epsilon 1} \frac{P \epsilon}{k} + c_{\epsilon 3} \frac{G}{\sqrt{\frac{k}{\bar{u}_3^2}}} \frac{\epsilon}{k} + c_{\epsilon} \left(\frac{k \bar{u}_3^2 \epsilon}{\epsilon} \right)_{,3} - c_{\epsilon 2} \frac{\epsilon^2}{k} \quad (3.110)$$

3.5.2 Algebraic equations

(a) Reynolds stresses: The following expressions for the non-zero components of reynolds stress tensor have been deduced from equation (3.106)

$$\begin{aligned} \frac{\bar{u}_1^2}{k_1} = & \left(\frac{2Rt}{3} (3 - 2c_2 + c_2' c_2 f(\frac{1}{x_3})) - \frac{2(1 - c_1)}{3} + c_1' \frac{\bar{u}_3^2}{k} f(\frac{1}{x_3}) \right. \\ & - \frac{2}{3} \frac{Rf}{Rf - 1} Rt (-c_3 + 2c_3' c_3 f(\frac{1}{x_3}) + 3 - 2c_2 + c_2 c_2' f(\frac{1}{x_3})) / \\ & \left. (c_1 + Rt - 1) \right) \end{aligned} \quad (3.111)$$

$$\begin{aligned} \frac{\bar{u}_2^2}{k_2} = & \left(\frac{2Rt}{3} (c_2 + c_2' c_2 f(\frac{1}{x_3})) - \frac{2(1 - c_1)}{3} - \frac{2}{3} \frac{Rf}{1 - Rf} Rt (c_3 - \right. \\ & c_2 - c_2 c_2' f(\frac{1}{x_3}) - 2c_3' c_3 f(\frac{1}{x_3})) + c_1' \frac{\bar{u}_3^2}{k} f(\frac{1}{x_3}) \left. \right) / (c_1 + Rt - 1) \end{aligned} \quad (3.112)$$

$$\begin{aligned} \frac{\bar{u}_3^2}{k_3} = & \left(\frac{2Rt}{3} (c_2 - 2c_2 c_2' f(\frac{1}{x_3})) - \frac{2(1 - c_1)}{3} - \frac{2}{3} \frac{Rf}{1 - Rf} Rt (3 - \right. \\ & 2c_3 + 4c_3' c_3 f(\frac{1}{x_3}) - c_2 + 2c_2' c_2 f(\frac{1}{x_3})) \left. \right) / (c_1 + 2c_1' f(\frac{1}{x_3}) \\ & + Rt - 1) \end{aligned} \quad (3.113)$$

$$\begin{aligned} \frac{\bar{u}_1 \bar{u}_3}{k} = & - \frac{\bar{u}_3^2 \bar{U}}{\epsilon} {}_{1,3} (1 - c_2 + \frac{3c_2' c_2}{2} f(\frac{1}{x_3})) + \frac{g}{\theta_m} \frac{\bar{u}_1 \theta}{\epsilon} \\ & (1 - \frac{3c_3' c_3}{2} f(\frac{1}{x_3})) / (Rt + g_1 - 1 + \frac{3c_1' f(\frac{1}{x_3})}{2}) \end{aligned} \quad (3.114)$$

where $Rt = -\bar{u}_1 \bar{u}_3 \bar{U}_{1,3} (1 - Rf) / \epsilon$, $Rf = \frac{g}{\theta_m} \frac{\bar{u}_3 \theta}{\bar{u}_1 \bar{u}_3 \bar{U}_{1,3}}$

and $f(\frac{1}{x_3}) = \frac{k^{3/2}}{3.28 \epsilon x_3}$.

(b) Scalar fluxes

(i) Heat fluxes: The non-zero components of the heat flux vector $\overline{u_i \theta}$ are:

$$\overline{u_1 \theta} = \frac{k}{\epsilon} (-\overline{u_1 u_3} \overline{\theta}_{,3} + \overline{u_3 \theta} \overline{u}_{1,3} (c_{2c} - 1)) / (0.5(Rt - 1) + c_{1c}) \quad (3.115)$$

$$\overline{u_3 \theta} = -\frac{k \overline{u_3^2} \overline{\theta}_{,3}}{\epsilon} / ((c_{1c} + c'_{1c} f(\frac{1}{x_3}) + \frac{1}{2}(Rt - 1) + \frac{g_c}{\theta_m} \left(\frac{k}{\epsilon}\right)^2 \overline{\theta}_{,3})$$

$$(1 - c_{3c} + c'_{3c} c_{3c} f(\frac{1}{x_3})) \quad (3.116)$$

(ii) Concentration fluxes: The components of the turbulent concentration vector read

$$\overline{u_1 c} = \frac{k}{\epsilon} (-\overline{u_1 u_3} \overline{c}_{,3} + \overline{u_3 c} \overline{u}_{1,3} (c_{2c} - 1)) / (0.5(Rt - 1) +$$

$$a_3 c_{1c} \frac{k^{3/2}}{\epsilon \delta_c}) \quad (3.117)$$

$$\overline{u_2 c} = \frac{k \overline{u_2^2} \overline{c}_{,2}}{\epsilon} / (a_3 c_{1c} \frac{k^{3/2}}{\epsilon \delta_c} + 0.5(Rt - 1)) \quad (3.118)$$

$$\overline{u_3 c} = -\frac{k \overline{c}_{,3}}{\epsilon} (\overline{u_3^2} + a' \frac{k}{\epsilon} \frac{g_c \overline{u_3 \theta}}{\theta_m} (1 - c_{3c} + c'_{3c} c_{3c} f(\frac{1}{x_3}))) /$$

$$(a_3 c_{1c} \frac{k^{3/2}}{\epsilon \delta_c} + c'_{1c} f(\frac{1}{x_3}) + 0.5(Rt - 1) + a' \frac{g_c \overline{\theta}_{,3}}{\theta_m} \frac{k^2}{\epsilon^2} (1 -$$

$$c_{3c} + c'_{3c} c_{3c} f(\frac{1}{x_3})) \quad (3.119)$$

CHAPTER 4

SOLUTION PROCEDURE

This chapter is devoted to the presentation of the numerical solution procedure employed in the present investigation. In section 4.1 the finite difference grid and coordinate system used is described. Section 4.2 deals with the transformation of the governing partial differential equations from the cartesian frame of reference in which they were assembled in chapters 2 and 3 to the new coordinate system more suitable for the numerical procedure. The equations are then cast, under certain assumptions, into their equivalent finite difference forms in section 4.3. In sections 4.4 and 4.5 the methods of solving the resultant finite difference equation and the algebraic equation for the turbulence fluxes (3.111) to (3.116) are respectively presented. In two sections 4.6 and 4.7 which follow the boundary and initial conditions employed are respectively given. Finally, a brief discussion of the sources of errors involved in the procedure is continued in section 4.8.

4.1 Finite-difference grid

In numerical solution procedures values of the dependent variables are calculated at discrete points in the flow domain. For ease of organisation of the calculations, the domain is imagined to be overlaid by a regular computational grid which defines the forementioned points or 'nodes' as

they are often called.

The formulation of a 'proper' grid is a prerequisite to an efficient and accurate numerical solution. In general the following define what is meant by 'proper':

- (i) The points should be closely spaced in regions where large gradients of the variables are expected and more widely spaced elsewhere.
- (ii) The overall shape of the grid should conform to the shape of the domain thus minimising the number of grid points required and also facilitating application of boundary conditions.
- (iii) One set of grid lines should preferably align with the direction of the flow, to reduce numerical diffusion (c.f. Gosman et al (1969)).

A further requirement is that the distribution of the variables on the grid should be such as to minimise the amount of interpolation (which at times is inevitable) required and hence computational effort.

A coordinate system that could (approximately) satisfy such requirements in two dimensional boundary layer flows is the non-dimensionalised stream function and x_1 coordinate system employed by Patankar and Spalding (1967). The drawback, however, of such a system is that it cannot be extended to three dimensional flows[‡] (for then the relation between

*Here it is assumed that the grid would be formed by co-ordinate lines.

[‡]Although in the present study the flow field is restricted to be two-dimensional, it was desired to develop a procedure that could eventually be extended to three dimensional flows.

stream-function and spatial distance ceases to be one to one).

Another system that partially fulfills the above requirements and is also applicable to three dimensional problems is defined by

$$\alpha_1 = x_1, \alpha_2 = x_2/\Delta_2, \alpha_3 = x_3/\Delta_3 \quad (4.1)$$

where Δ_2 and Δ_3 are typical length scales of the domain of interest (which may vary with x_1) in the x_2 and x_3 directions respectively.

A further factor which must be considered is that in atmospheric dispersion calculations the use of a single grid for both concentration and hydrodynamic fields may often be uneconomical, because in the initial stages of the plume development the characteristic dimensions of the plume cross-section may be several orders of magnitude smaller than the dimensions of the boundary layer. Consequently a grid suitable to resolve the flow field would be far too coarse to resolve the concentration field in the plume, while the fineness of the grid required for the latter would be unnecessary for the flow field. For these reasons independent grids are employed for the two fields in the present study.

The hydrodynamic and temperature fields being at present two-dimensional may be defined in two-dimensional coordinate system $\xi_1 \sim \xi_2$ which is defined as:

$$\xi_1 = x_1 \quad (4.2a)$$

$$\xi_3 = x_3/\delta \quad (4.2b)$$

where δ is the thickness of the boundary layer.

The coordinate system used for the concentration grid is:

$$\eta_1 = x_1 \quad (4.3a)$$

$$\eta_2 = x_2/X_2 \quad (4.3b)$$

$$\eta_3 = (x_3 - x_3^1)/(X_3^h - x_3^1) \quad (4.3c)$$

where X_2 is the lateral width of the plume and X_3^h and x_3^1 are the vertical distances from the ground to the upper and lower boundaries of the plume respectively. A view of the two grid system is shown in figures 4.1a and 4.1b.

The storage location of the variable $\bar{\theta}$, k and ϵ is at the nodes of the 'hydrodynamic' grid*, while the velocities $\bar{U}_1$ and $\bar{U}_3$ are placed mid-way between these nodes, on grid lines $\xi_1 = \text{constant}$ and $\xi_3 = \text{constant}$, as shown in figure 4.1a where the vertical and horizontal arrows denote $\bar{U}_1$ and $\bar{U}_3$ location respectively. This 'staggered' arrangement of variables facilitates the calculation of the convection fluxes

*Henceforth the hydrodynamic grid will be referred to as 'grid 1' and the concentration one as 'grid 2'.

of the scalars $\bar{\theta}$, k and ϵ .

The concentrations are calculated at the grid 2 nodes, and the stream-wise and vertical velocities required for these calculations are stored at intervening locations in the manner of grid 1 arrangement. The stream-wise velocities on grid 2 are obtained by linear interpolation and the vertical velocities are then determined from the local mass continuity requirement. Modification to this practice is made at near ground locations when concentration grid nodes fall below nodes on grid 1 adjacent to the ground. In such cases the velocity on grid 2 is calculated from the logarithmic law of the wall. (Further details are given in section 4.6.1).

4.2 Transformation of the differential equations to η_1, η_2, η_3 and ξ_1, ξ_3 coordinates

From differential calculus and relations (4.3a), (4.3b) and (4.3c) we get the following relations between differentials in the old and new coordinate frames:

$$\left. \frac{\partial}{\partial x_1} \right)_{x_2, x_3} = \left. \frac{\partial}{\partial \eta_1} \right)_{\eta_2, \eta_3} - \left. \frac{\partial}{\partial \eta_2} \right)_{\eta_1, \eta_3} \frac{dx_2}{dx_1} \frac{\eta_2}{x_2} - \left. \frac{\partial}{\partial \eta_3} \right)_{\eta_1, \eta_2} \left[\frac{dx_3}{dx_1} \frac{\eta_3}{x_3} + \frac{dx_3^1}{dx_1} \frac{1}{x_3} \right] \quad (4.4)$$

$$\left. \frac{\partial}{\partial x_2} \right)_{x_1, x_3} = -\frac{1}{x_2} \left. \frac{\partial}{\partial \eta_2} \right)_{\eta_1, \eta_3} \quad (4.5)$$

$$\left. \frac{\partial}{\partial x_3} \right)_{x_1, x_2} = \frac{1}{x_3} \left. \frac{\partial}{\partial \eta_3} \right)_{\eta_1, \eta_2} \quad (4.6)$$

where $X_3 = X_3^h - X_3^1$.

Thus in $\eta_1 \eta_2 \eta_3$ coordinates the concentration equation (2.49) becomes:

$$\begin{aligned} \frac{\partial \bar{U}_1 \bar{C}}{\partial x_1} - \frac{\eta_2}{X_2} \frac{dx_2}{d\eta_1} \frac{\partial \bar{U}_1 \bar{C}}{\partial \eta_2} - \frac{\eta_3}{X_3} \frac{dx_3}{d\eta_1} \frac{\partial \bar{U}_1 \bar{C}}{\partial \eta_3} - \frac{1}{X_3} \frac{dx_3^1}{d\eta_1} \frac{\partial \bar{U}_1 \bar{C}}{\partial \eta_3} \\ + \frac{1}{X_3} \frac{\partial \bar{U}_3 \bar{C}}{\partial \eta_3} = - \frac{1}{X_2} \frac{\partial \bar{u}_2 \bar{C}}{\partial \eta_2} - \frac{1}{X_3} \frac{\partial \bar{u}_3 \bar{C}}{\partial \eta_3} + \bar{S}_c \end{aligned} \quad (4.7)$$

Similarly the equations of continuity (2.46), momentum (2.47), energy (2.48), turbulence kinetic energy (3.109) and its dissipation rate (3.110) are transformed to:

$$\frac{\partial \bar{U}_1}{\partial \xi_1} - \frac{\xi_3}{\delta} \frac{d\delta}{d\xi_1} \frac{\partial \bar{U}_1}{\partial \xi_3} + \frac{1}{\delta} \frac{\partial \bar{U}_3}{\partial \xi_3} = 0 \quad (4.8)$$

$$\frac{\partial \bar{U}_1 \bar{U}_1}{\partial \xi_1} - \frac{\xi_3}{\delta} \frac{d\delta}{d\xi_1} \frac{\partial \bar{U}_1 \bar{U}_1}{\partial \xi_3} + \frac{1}{\delta} \frac{\partial \bar{U}_3 \bar{U}_1}{\partial \xi_3} = - \frac{1}{\delta} \frac{\partial \bar{u}_1 \bar{u}_3}{\partial \xi_3} \quad (4.9)$$

$$\frac{\partial \bar{U}_1 \bar{\theta}}{\partial \xi_1} - \frac{\xi_3}{\delta} \frac{d\delta}{d\xi_1} \frac{\partial \bar{U}_1 \bar{\theta}}{\partial \xi_3} + \frac{1}{\delta} \frac{\partial \bar{U}_3 \bar{\theta}}{\partial \xi_3} = - \frac{1}{\delta} \frac{\partial \bar{u}_3 \bar{\theta}}{\partial \xi_3} \quad (4.10)$$

$$\frac{\partial \bar{U}_1 k}{\partial \xi_1} - \frac{\xi_3}{\delta} \frac{d\delta}{d\xi_1} \frac{\partial \bar{U}_1 k}{\partial \xi_3} + \frac{1}{\delta} \frac{\partial \bar{U}_3 k}{\partial \xi_3} = - \frac{1}{\delta} \frac{\bar{u}_1 \bar{u}_3}{\bar{\theta}_m} \frac{\partial \bar{U}_1}{\partial \xi_3} + g \frac{\bar{\theta} \bar{u}_3}{\bar{\theta}_m}$$

$$+ \frac{c_s}{\delta^2} \frac{\partial}{\partial \xi_3} \frac{k}{\bar{\epsilon}} \frac{\bar{u}_3^2}{\bar{\epsilon}} \frac{\partial k}{\partial \xi_3} - \epsilon$$

$$(4.11)$$

$$\begin{aligned} \frac{\partial \bar{U}_1 \epsilon}{\partial \xi_1} - \xi_3 \frac{d\delta}{d\xi_1} \frac{\partial \bar{U}_1 \epsilon}{\partial \xi_3} + \frac{1}{\delta} \frac{\partial \bar{U}_3 \epsilon}{\partial \xi_3} = -c_{\epsilon 1} \frac{\bar{u}_1 \bar{u}_3}{\delta} \frac{\partial \bar{U}_1 \epsilon}{\partial \xi_1} \frac{1}{k} \\ + c_{\epsilon 3} g \frac{\bar{\theta} \bar{u}_3}{\theta_m} \sqrt{\frac{k}{\bar{u}_3^2 k}} \frac{\epsilon}{\delta} + c_{\epsilon} \frac{\partial}{\partial \xi_3} \left(\frac{k \bar{u}_3^2 \partial \epsilon}{\partial \xi_3} \right) - c_{\epsilon 2} \frac{\epsilon^2}{k} \end{aligned} \quad (4.12)$$

Equations (4.9) to (4.12) are all of the general form:

$$\frac{\partial \bar{U}_1 \phi}{\partial \xi_1} - \xi_3 \frac{d\delta}{d\xi_1} \frac{\partial \bar{U}_1 \phi}{\partial \xi_3} + \frac{1}{\delta} \frac{\partial \bar{U}_3 \phi}{\partial \xi_3} = P^\phi - \frac{1}{\delta^2} \frac{\partial}{\partial \xi_3} \left(\frac{\Gamma_3^\phi \partial \phi}{\partial \xi_3} \right) \quad (4.13)$$

where ϕ is any of the variables $\bar{U}_1$, θ , k or ϵ , P^ϕ is the source and/or sink of ϕ and Γ_3^ϕ is the diffusivity. The definitions of P^ϕ and Γ_3^ϕ corresponding to the different variables are summarised in Table 4.1.

It is important to note that the 'diffusivities' Γ_3^ϕ are employed here merely for convenience in the numerical calculations and do not represent a departure from the original physical model described in Chapter 3. The Γ_3^ϕ 's are in fact calculated from knowledge of the turbulent fluxes and not vice-versa*; i.e.

$$\Gamma_i^\phi = -\frac{\overline{u_i \phi}}{\partial \phi / \partial x_i} \quad (4.14)$$

where $\overline{u_i \phi}$'s are calculated from the equations given in section 3.5.2.

* Similar equations exist to calculate K_2 and K_3 for the concentration calculations.

4.3 Finite difference equations

The finite difference equations are obtained by integrating the partial differential equations over small volume elements termed 'control volumes'. The latter are defined as surrounding the grid nodes such that the boundaries of the control volume lie mid-way between the grid lines. An exception to the foregoing definition is made for those grid nodes adjacent to the physical boundaries; there the outer boundary of the control volume surrounding each such node is made to coincide with the physical boundary, as illustrated in figure 4.1a.

This 'micro-integral' technique is here preferred to the method of Taylor series expansion, because it is easier to ensure that the resultant finite-difference equations satisfy the relevant conservation laws.

4.3.1 Finite differencing schemes

In formulating the finite difference equations the average values of the dependent variables are required at the surfaces of the control volumes. Two practices are usually followed for this purpose (c.f. Gosman et al (1969)); the first is to assume that the variable in question varies linearly between the two nodes bracketing the surface in question and hence the value of the variable at the surface is the weighted average of the nodal values; this procedure is usually referred to as 'central differencing'. The second practice is to employ 'up wind-differencing', in which it is assumed that the value at the control volume surface is equal to that at the upwind node.

In an investigation carried out to determine which of the two differencing schemes is superior, Spalding (1970) found by comparing finite-difference approximations and the exact solution to a one-dimensional convection diffusion problem, that when the absolute value of the grid Peclet number Pe_m is less than 2, where the latter is defined as:

$$Pe_m = G_m \Delta x_m / \Gamma_m$$

with G_m denoting the mass flux at the boundary m (e.g. $m = n, s, \dots$), Δx_m the nodal separation (surrounding boundary m) and Γ_m the appropriate diffusivity, central differencing is more accurate, while for $|Pe_m| > 2$ upwind differencing is superior. Consequently Spalding (1970) (see also Runchal (1972)) suggested that a 'hybrid' scheme should be used whereby central differencing is adopted for $|Pe_m| > 2$ and upwind differencing is used otherwise. In the recommended form of upwind differencing in this scheme the diffusion contribution is neglected.

In the present flow situation, the grid Peclet number in the main flow direction (i.e. $G_d \Delta x_d / \Gamma_d$) is, consistent with the boundary layer assumption, expected to be always greater than 2 (provided Δx_d is not too small) and hence upwind differencing is employed in this direction. In the vertical and lateral* directions; however, the hybrid scheme

*Used only for the concentration equation as the flow equation is two dimensional.

is employed.

4.3.2 Concentration equation

The finite difference form of the concentration equation (4.7) is obtained by integrating the latter over the control volume shown in figure 4.3. By introduction of the differencing practices mentioned earlier the following equation for the concentration at point P; C_p in terms of the neighbouring concentrations $C_N, C_N \dots$ etc (full details of the derivation are given in appendix D1) is obtained

$$(a'_p - S_p)C_p = a_u C_u + a_n C_N + a_s C_S + a_e C_E + a_w C_W + S_U \quad (4.15)$$

where the $a_u, a_n \dots$ etc. are combined convection/diffusion coefficients at the different boundaries and are defined as:

$$a_u = G_u \quad (4.16)$$

$$a_n = \begin{cases} G_n A_n & \text{Pe}_n < -2 \\ (1/\text{Pe}_n - \frac{1}{2}) G_n A_n & -2 \leq \text{Pe}_n \leq 2 \\ 0 & \text{Pe}_n > 2 \end{cases} \quad (4.17)$$

$$a_s = \begin{cases} 0 & \text{Pe}_s < -2 \\ (1/\text{Pe}_s + \frac{1}{2}) G_s A_s & -2 \leq \text{Pe}_s \leq 2 \\ G_s A_s & \text{Pe}_s > 2 \end{cases} \quad (4.18)$$

$$a_e = \begin{cases} G_e A_e & Pe_e < -2 \\ (1/Pe_e + \frac{1}{2}) G_e A_e & -2 \leq Pe_e \leq 2 \\ 0 & Pe_e > 2 \end{cases} \quad (4.19)$$

$$a_w = \begin{cases} 0 & Pe_e < -2 \\ (1/Pe_w - \frac{1}{2}) G_w A_w & -2 \leq Pe \leq 2 \\ G_w A_w & Pe > 2 \end{cases} \quad (4.20)$$

The A's here are the areas of the control-volume boundaries (the full definitions of the G's and A's are given in appendix D1). Further

$$a'_p = a_u + a_n + a_s + a_e + a_w \quad (4.21)$$

and S_u and S_p are defined by the following linearisation of the source terms $\bar{S}_c$

$$\iiint \bar{S}_c d\epsilon_1 d\epsilon_2 d\epsilon_3 = S_p C_p + S_u \quad (4.22)$$

Although S_p and S_u are determined in part by the form of $\bar{S}_c$, they are not unique and can be formulated so as to aid numerical stability of the solution. In the present study S_c is zero and hence S_p and S_u are zero; this condition is altered near boundaries when a pollutant flux exists to/from the boundary as expounded in section 4.6.2.

4.3.3 Flow equations

A similar procedure is applied to the general flow

equation (4.13) with the integration now performed over the control volume shown in figure 4.4. The following equation is obtained for ϕ_P :

$$(a_P^\phi - S_P^\phi) \phi_P = a_u^\phi \phi_U + a_n^\phi \phi_N + a_s^\phi \phi_S + S_U^\phi \quad (4.23)$$

where a_s' , S_P^ϕ and S_U^ϕ have similar significance as those described earlier but for a two dimensional variable ϕ . These are defined by

$$a_u^\phi = G_u A_u \quad (4.24)$$

$$a_n^\phi = \begin{cases} G_n A_n & \text{Pe}_n^\phi < -2 \\ (1/\text{Pe}_n^\phi - \frac{1}{2}) G_n A_n & -2 \leq \text{Pe}_n^\phi \leq 2 \\ 0 & \text{Pe}_n^\phi > 2 \end{cases} \quad (4.25)$$

$$a_s^\phi = \begin{cases} 0 & \text{Pe}_s^\phi < -2 \\ (1/\text{Pe}_s^\phi + \frac{1}{2}) G_s A_s & -2 \leq \text{Pe}_s^\phi \leq 2 \\ G_s A_s & \text{Pe}_s^\phi > 2 \end{cases} \quad (4.26)$$

where the superscript ϕ defines the different variables (i.e. $\bar{U}_1$, $\bar{\theta}$ etc.). The definitions of the source coefficients for the different variables are as follows:

$$S_P^U = S_U^U = S_P^\theta = S_U^\theta = 0$$

$$S_U^k = (P + G) \Delta \xi_1 \Delta \xi_3 \delta \quad (4.27a)$$

$$S_U^\epsilon = C_{\epsilon 1} P_\epsilon \epsilon \Delta \xi_1 \Delta \xi_3 \delta / k \quad (4.27b)$$

$$S_p^k = -\epsilon \Delta \xi_1 \Delta \xi_3 \delta / k \quad (4.28a)$$

$$S_p^e = -c_{\epsilon 2} \epsilon \Delta \xi_1 \Delta \xi_3 \delta / k \quad (4.28b)$$

Integration of the continuity equation over the same control volume gives the following equation for $(\bar{U}_3)_p$

$$(U_3)_1 = (\bar{U}_3)_s + ((\bar{U}_1)_p - (\bar{U}_1)_u) \frac{\delta \Delta \xi_3}{\Delta \xi_1} + ((U_1 \xi_3)_n - (\bar{U}_1 \xi_3)_s) \frac{d\delta}{dx} - (\bar{U}_1)_p \frac{d\delta}{d\xi_1} \Delta \xi_3 \quad (4.29)$$

4.4 Method of solving finite difference equations

It can be seen from equation (4.15) that the model value of any variable at a point P is related to all neighbouring points with the exception of the downstream one. The upstream value C_u is assumed to be known so that unknowns are C_p and its neighbours in the same plane. It follows that if one such equation is written for each node in a cross-stream plane there results a set of simultaneous equations for the values in that plane.

Equation (4.15) is expressed for the purpose of solution in the following alternative notation:

$$(aP - SP)_{i,j} C_{i,j,k} = a_n{}_{i,j} C_{i,j+1,k} + a_s{}_{i,j} C_{i,j-1,k} + a_e{}_{i,j} C_{i+1,j,k} + a_w{}_{i,j} C_{i-1,j,k} + a_u{}_{i,j} C_{i,j,k-1} + S U_{i,j} \quad (4.30)$$

where the suffixes i and j denote the grid node location in the lateral and vertical directions respectively (see figure 4.2) and k specifies the cross-stream plane, as shown in

figure 4.1, the coefficients a_p , a_n etc. have the same meaning as a_p, a_n appearing in equation (4.15).

Similarly equation (4.23) is expressed as

$$(a_p - SP^\phi)_j \phi_{j,k} = a_n \phi_{j,k} + a_s \phi_{j-1,k} + a_u \phi_{j,k-1} + SU_j^\phi \quad (4.31)$$

The solution of equations (4.30) and (4.31) proceeds in a stepwise manner starting from the upstream end of the integration domain (starting from $k = 2$) and proceeding step by step downstream. For each step the calculation proceeds as follows:

- (i) Calculate k , ϵ and θ from equation (4.31) using upstream values of $\bar{U}_3$, the Γ_ϕ 's and the source coefficients (i.e. Sp and SU).
- (ii) From the just-obtained values of k , ϵ and θ , calculate the turbulent fluxes $\overline{u_1 u_3}$, $\overline{u_3 \theta}$, $\overline{u_3 c}$ etc. and hence the Γ 's from equation (4.14).
- (iii) Solve for $\bar{U}_1$ from equation (4.31) using upstream values of U_3 .
- (iv) Apply (4.29) to obtain $\bar{U}_3$.
- (v) Interpolate to get values of $\bar{U}_1$, K_2 , K_3 on the concentration grid.
- (vi) Solve for $\bar{C}$ from equation (4.30). This completes the sequences.

Strictly speaking the coupling between the equation for $\bar{U}_1$, k , ϵ and $\bar{\theta}$ could require iteration over the sequence (i) to (iv): however because the boundary-layer character of the flow implies slow variation in the stream-wise direction the need for iteration is avoided by

appropriately restricting the size of the forward step.

For the solution of equation (4.30) in a given cross-sectional plane Gauss elimination method (c.f. Donn and McCracken (1972)) is applied to solve for the concentration along each vertical grid line i with the values of $\bar{C}$ having subscripts $i-1$ and $i+1$ temporarily assumed as known. Once values of line i is known solution proceeds to the next vertical line $i+1$ and so on until all the concentration values lying in the cross-stream plane has been obtained. This concludes what is known as a 'sweep'. Because the method of solution is iterative more than one sweep is usually required to obtain a satisfactory solution; the satisfactoriness being assessed by ways which will be mentioned shortly. However in the case of the variables $\bar{U}_1$, $\bar{\theta}$, k or ε the absence of lateral neighbouring lines renders one application of the Gauss elimination method sufficient for the solution.

A sufficient condition for a numerical stability in the iterative solution of (4.30) (according to Donn and McCracken (1977)) is that for a values of i and j

$$|(ap - sp)_{i,j}| \geq |(an + as + ae + aw)_{i,j}| \quad (4.32)$$

with strict inequality for at least one j . With the present formulation the above condition is always fulfilled.

4.5 Solution of the algebraic turbulent flux equations

The algebraic flux equations, which are non-linear and simultaneous, may be recast into the following forms

$$\bar{u}_1^2 = \frac{2k}{3}(\gamma_1 + \gamma_3 + 1.5\gamma_5\bar{u}_3^2/k + \frac{RtRf}{1-Rf} \gamma_4)/\gamma_2 \quad (4.33)$$

$$\bar{u}_2^2 = \frac{2k}{3}(\gamma_9 + \gamma_1 - \frac{RtRf}{1-Rf} \gamma_{10} + 1.5\gamma_5\bar{u}_3^2/k)/\gamma_2 \quad (4.34)$$

$$\bar{u}_3^2 = \frac{2k}{3}(\gamma_1 + \gamma_6 - \frac{RtRf}{1-Rt} \gamma_7)/\gamma_8 \quad (4.35)$$

$$\frac{\partial \bar{u}_1 \bar{u}_3}{\partial x_3} = -\frac{k^2}{\epsilon \partial U_1} (\gamma_{11} \frac{\bar{u}_3^2}{k} + \frac{RtRf}{1-Rf} (\gamma_{14} - Pr_t) \gamma_{12} / \gamma_{15}) / \gamma_{13} \quad (4.36)$$

$$Pr_t = \gamma'' (\gamma_{11} + \frac{RfRt}{1-Rf} \frac{k}{\bar{u}_3^2} \frac{\gamma_{12}\gamma_{14}}{\gamma_{15}}) / \{\gamma_{13} (1 - \frac{RtRf}{1-Rf} \frac{k}{\bar{u}_3^2} c_\theta \gamma') + \gamma'' \frac{RtRf}{1-Rf} \frac{k}{\bar{u}_3^2} \gamma_{12} / \gamma_{15}\} \quad (4.37)$$

where

$$\gamma_1 = c_1 - 1$$

$$\gamma_2 = \gamma_1 + Rt$$

$$\gamma_3 = (3 - 2c_2 + c_2 c_2' f(1/x_3)) Rt$$

$$\gamma_4 = 3 - 2c_2 - c_3$$

$$\gamma_5 = c_1' f(1/x_3)$$

$$\gamma_6 = (c_2 - 2c_2 c_2' f(1/x_3)) Rt$$

$$\gamma_7 = (3 - 2c_3 - c_2) + 4c_3 c_3' f(1/x_3) + 2c_2 c_2' f(1/x_3)$$

$$\gamma_8 = c_1 - 1 + 2\gamma_5 + Rt$$

$$\gamma_9 = (c_2 + c_2 c_2' f(1/x_3)) Rt$$

$$\gamma_{10} = (c_3 - c_2 - c_2 c_2' f(1/x_3) - 2c_3 c_3' f(1/x_3))$$

$$\gamma_{11} = 1 - c_2 + 1.5c_2 c_2' f(1/x_3)$$

$$\gamma_{12} = 1 - c_3 + 1.5c_3c'_3f(1/x_3)$$

$$\gamma_{13} = \gamma_2 + 1.5c'_1f(1/x_3)$$

$$\gamma_{14} = c_{2c} - 1$$

$$\gamma_{15} = 0.5Rt - 0.5 + c_{1c}$$

$$\gamma' = 1 - c_{3c} + c_{3c}c'_{3c}f(1/x_3)$$

$$\gamma'' = c_{1c} + c'_{1c}f(1/x_3) + \gamma_{15}$$

It should be noted that the original equation (3.116) for $\overline{u_3\theta}$ has been transformed into one for Pr_t , as it is this variable that directly appears in the present formulation for $\overline{u_1u_3}$.

Solution of equations (4.33) to (4.37) is achieved by a successive-substitution method the sequence of which is as follows:-

- (i) Equation (4.35) is solved for $\overline{u_3^2}$ with upstream values of Rt and Rf inserted.
- (ii) Equations (4.33), (4.34) and (4.37) are then solved for $\overline{u_1^2}$, $\overline{u_2^2}$ and Pr_t respectively using the just-calculated value of $\overline{u_3^2}$ and upstream values of Rf and Rt .
- (iii) The equation for $\overline{u_1u_3}$ is then solved using newly-obtained variables from the previous step.
- (iv) The parameters Rt and Rf are computed the latter being obtained from:

$$Rf = g \overline{\theta}_{,3} / Pr_t \overline{u_{1,3}^2} \theta_m \quad (4.38)$$

Because of non-linearity and coupling of the equations ideally the whole of the above sequence should be repeated to converge, however as mentioned, by taking sufficiently

small forward steps a sufficiently accurate solutions can be obtained without iteration.

Once the turbulent stresses are calculated the concentration fluxes $\overline{u_2 c}$ and $\overline{u_3 c}$ are obtained directly from equations (3.118) and (3.119) respectively: these are then available to calculate K_2 and K_3 for use in the concentration solution.

The above method of solution was found to be successful in all cases investigated except when relatively severe stable stratification (i.e. $Rf \sim 0.08$) was specified. In such circumstances numerical instabilities were encountered and the following different approach was adopted.

Inspection of equations (4.33) to (4.37), (3.118) and (3.119) reveals that $\overline{u_1^2}$, $\overline{u_2^2}$, $\overline{u_2 c}$ and $\overline{u_3 c}$ are all dependent on $\overline{u_1 u_3}$, Pr_t and $\overline{u_3^2}$ but not vice-versa; also the latter three variables are coupled to each other*. Hence the equations for $\overline{u_1 u_3}$, Pr_t and $\overline{u_3^2}$ may be simultaneously solved until a converged solution is obtained, and then $\overline{u_1^2}$, $\overline{u_2^2}$, $\overline{u_2 c}$ and $\overline{u_3 c}$ may be directly calculated.

Solution of the coupled equations is obtained by a modified Newton-Raphson method (c.f. Stark (1970)). Briefly this entails the following: equations (4.33), (4.36) and (4.37) are rearranged, with the aid of (4.38), respectively to the forms[‡]:

*Note that, since Rt and Rf are dependent on $\overline{u_1 u_3}$ and Pr_t the equation of $\overline{u_1 u_3}$ and Pr_t are non-linear.

[‡] F_1 , F_2 and F_3 are given in appendix D2.

$$F_1(\overline{u_1 u_3}, \overline{u_3^2}, Pr_t) = 0 \quad (4.40)$$

$$F_2(\overline{u_1 u_3}, \overline{u_3^2}, Pr_t) = 0 \quad (4.41)$$

$$F_3(\overline{u_1 u_3}, \overline{u_3^2}, Pr_t) = 0 \quad (4.42)$$

The following iteration formula for $(\overline{u_3^2})_m$ is then employed:

$$(\overline{u_3^2})_m = (\overline{u_3^2})_{m-1} + \left[\frac{F_1}{\partial F_1 / \partial \overline{u_3^2}} \right]_{m-1} \quad (4.43)$$

where the suffix m denotes the current iterate and (m-1) denotes the value from the previous iteration. Similarly $\overline{u_1 u_3}$ and Pr_t are calculated respectively from

$$(\overline{u_1 u_3})_m = (\overline{u_1 u_3})_{m-1} + \left[\frac{F_2}{\partial F_2 / \partial \overline{u_1 u_3}} \right]_{m-1} \quad (4.44)$$

$$(Pr_t)_m = (Pr_t)_{m-1} + \left[\frac{F_3}{\partial F_3 / \partial Pr_t} \right]_{m-1} \quad (4.45)$$

These formulae are repeatedly applied until convergence is obtained, as assessed by the criteria

$$\left| \frac{F_1 / \overline{u_1^2} \partial F_1}{\partial \overline{u_1^2}} \right| < 0.01, \quad \left| \frac{F_2 / \overline{u_1 u_3} \partial F_2}{\partial \overline{u_1 u_3}} \right| < 0.01$$

and $\left| \frac{F_3 / Pr_t \partial F_3}{\partial Pr_t} \right| < 0.01 \quad (4.46)$

4.6 Boundary conditions and their implication

For the flow and temperature calculations boundary conditions on the associated variables (i.e. U , θ , k and ϵ) need to be specified at the upper or 'free' surface of the boundary layer and at ground level. The concentration calculations require specifications at 4 boundaries i.e. at the upper and lower surfaces of the grid (the latter can be above or at ground level) as defined by the heights X_3^h and X_3^l respectively, the plane of symmetry ($X_2 = 0$) which passes through the centre of the source and the vertical outer boundary defined by the X_2 coordinate.

The conditions employed for the different variables and types of boundary are as follows.

4.6.1 Boundary conditions for hydrodynamic and energy equations

a) Free boundary: The values of all the variables ($\bar{U}_1$, $\bar{\theta}$, k and ϵ) are prescribed according to the specification of the problem. No further steps are required in order to apply such conditions.

b) Ground boundary: In the region close to a smooth wall three subranges may be distinguished (c.f. Hinze (1975)). Closest to the ground is a viscous sublayer where turbulence effects may be neglected; above this lies a buffer region wherein viscous and turbulence effects are important; and the uppermost layer is a fully turbulent region. Because the turbulence model in its present form is invalid in the first two zones (Re_1 is small and viscous effects are important) these regions are avoided by ensuring that the grid nodes closest to the ground are at a height greater

than $30\nu/u_*$ and making special modifications to the equations at these nodes, which will be described below.

A further incentive to avoid the near-wall region in the finite-difference calculations is that large gradients in the variables exist there, and thus to adequately resolve them would require a large number of grid nodes to be placed in this region.

Although for flows over completely rough walls* no viscous or buffer layers exist, close to the roughness elements separation of the flow may occur which would invalidate the boundary layer assumptions. Therefore, for rough walls it is also advantageous to avoid the near-wall region.

The treatment of the different variables at the ground boundary is as follows.

$\bar{U}_1$ velocity: The tangential velocity for a node adjacent to the ground $(\bar{U}_1)_p$, is obtained by solving the momentum equation there, but with the shear stress at the ground boundary calculated via the following relation:

$$\tau = \rho u_*^2$$

where the friction velocity u_* which, depends on thermal stratification (stable, neutral etc.) and the surface roughness is obtained from the following relations taken from Lumley and Panofsky (1964) and Monin and Yaglom (1977))

*Conventionally defined as corresponding to conditions for which $u_* k_s / \nu > 70$ where k_s is the height of the roughness elements (see for example Schlichting (1968)).

Rough wall:

$$u_* = \frac{\kappa(\bar{U}_1)_p}{\ln \left[\frac{(x_3)_p}{x_o} \right] + \beta' \frac{(x_3)_p}{L}} \quad (4.47)$$

Smooth wall:

$$u_* = \frac{\kappa(U_1)_p}{\ln \left[\frac{u_* (x_3)_p^E}{v} \right] + \beta' \frac{(x_3)_p}{L}} \quad (4.48)$$

Here L is the Monin-Obukhov length scale defined by:

$$L = \frac{u_*^3}{\frac{\kappa g}{\theta} \frac{H}{\rho c_p}} \quad (4.49)$$

β' and E are constants equal to 5 and 9.2 respectively, and the suffix P refers to conditions at the grid node adjacent to the ground.

It should be noted that in neutral flows $L = \infty$ and equation (4.47) and (4.48) then reduce to the well-known logarithmic laws for rough and smooth walls respectively.

In order to ensure that velocities calculated near the ground, experience the shear stress implied by equation (4.47) and (4.48) a 'false' viscosity μ_f (see Tatchel (1975)) is defined by:

$$\mu_f = (x_3)_p \tau / (\bar{U}_1)_p \quad (4.50)$$

This then serves as the viscosity at the boundary at ground level.

Boundary conditions for $\bar{\theta}$: Two types of boundary conditions for temperature are common. The first is when the surface heat flux (H) distribution is prescribed and the second is when the ground temperature variation is given. To apply the former, the coefficient as_2^θ for the energy equation (4.31) is set to zero and SU_2^θ is put equal to:

$$SU_2^\theta = H\Delta\xi_1/\rho c_p \quad (4.51)$$

When the boundary temperature is prescribed the following relations (taken from Lumley and Panofsky (1964) and Launder and Spalding (1972)) are employed to calculate T_*

Rough wall:

$$T_* = \frac{\kappa(\bar{\theta}_p - \theta_w)}{\text{Pr}_t \left[\ln \left[\frac{(x_3)_p}{x_o} \right] + \beta' \frac{(x_3)_p}{L} \right]} \quad (4.52)$$

Smooth wall:

$$T_* = \frac{\kappa(\bar{\theta}_p - \theta_w)}{\text{Pr}_t \left[\ln \left[\frac{E_\theta u_*(x_3)_p}{v} \right] + \beta' \frac{(x_3)_p}{L} \right]} \quad (4.53)$$

Here θ_w is the ground temperature and E_θ is a function of the laminar and turbulent Prandtl numbers (see Patankar and Spalding (1967), Launder and Spalding (1972)) which is

approximately equal to E for equal laminar and turbulent Prandtl numbers. For air close to the ground this is roughly the case ($Pr \approx 0.7$ and $Pr_t \approx 0.9$) and hence E_θ is taken equal to E .

From u_* and T_* a false diffusivity Γ_f is defined, in a fashion similar to a false viscosity:

$$\Gamma_f = (x_3)_p u_* T_* / (\bar{\theta}_p - \theta_w) \quad (4.54)$$

This is then taken as the diffusivity at ground level.

Boundary conditions for k and ϵ : Since as mentioned earlier, the equations for k and ϵ are not valid in the immediate vicinity of the ground, these variables are calculated at the grid node adjacent to the ground from special formulae given below.

According to the experimental data of Klebanoff (1954) k_p may be approximated by:

$$k_p \approx 4u_*^2 \quad (4.55)$$

where p lies in the region where the velocity obeys the logarithmic laws quoted earlier.

Close to a solid surface experimental evidence (see Townsend (1976)) reveals that the production and dissipation of k are the dominant terms in the transport equation (108) and hence the latter may be simplified to

$$\epsilon = -\overline{u_1 u_3} \frac{\partial \bar{U}_1}{\partial x_3} (1 - Rf) \quad (4.56)$$

Since in the region considered $-\overline{u_1 u_3} \approx u_*^2$ (Lumley and Panofsky (1964)); combination of equations (4.56) and (4.47) or (4.48) gives the following formula for the dissipation rate ϵ_p at P:

$$\epsilon_p = \frac{u_*^3}{\kappa} \left[\frac{1}{(\overline{x_3})_p} + \frac{\beta'}{\overline{L}} \right] (1 - Rf) \quad (4.57)$$

4.6.2 Boundary conditions for concentration

- (a) Top boundary: The value of the pollutant species concentration $\overline{c}$ is usually zero at the upper edges of the plume, a condition which may be directly prescribed.
- (b) Lower boundary: If the lower edge of the plume is above ground level (which may be the case for elevated sources) the concentration is set to zero, however if the edge reaches the ground the flux of the pollutant is specified; usually it will be zero unless phenomena such as deposition or absorption occur. The application of this condition in equation (4.30) is achieved by setting as_2 to zero and $SU_{i,2}$ to

$$SU_{i,2} = M_c \Delta \eta_1 \Delta \eta_2 X_2 \quad (4.58)$$

where M_c is the prescribed flux.

- (c) Plane of symmetry: The flux of $\overline{c}$ through this plane is by definition equal to zero and this is specified in the calculation by simply setting $aw_{2,j}$ (for all j) equal to zero.
- (d) Vertical outer boundary: The value of $\overline{c}$ at the lateral

edge of the plume is also known and is usually zero.

4.7 Initial conditions

The distribution of all variables must be specified at a starting plane. The measured values are used if these are available. In their absence however, a step function is assumed for the concentration field, i.e. the value of the concentration is assumed zero everywhere except at the location of the source where it is set equal to the value C_{in} , calculated from:

$$C_{in} = \frac{Q}{Q_{air} + Q} \quad (4.59)$$

where Q is the source strength and Q_{air} is the air flow rate flowing into the control volume containing the source.

For the boundary layer calculation universal similarity profiles shown in figures 4.5 and 4.6 are assumed to exist; from these the profiles of $\bar{U}_1$, k and ϵ can be obtained once the free stream value of $\bar{U}_1$, the boundary layer thickness and u_* are prescribed. The initial temperature profile, unless otherwise stated, is assumed to be uniform.

4.8 Accuracy of results

Errors in the predictions obtained from the foregoing procedure may stem from several sources. These are:

4.8.1 Physical modelling errors

These inaccuracies arise from imprecise mathematical

modelling of the physical processes occurring in the flow, particularly those associated with turbulence. They enter the calculation via the approximation inherent in the turbulence model employed.

Further sources of physical errors may arise due to uncertainties about the starting fields and/or the boundary conditions. These sources of inaccuracy are particularly likely to occur in simulations of full-scale field experiments, which are seldom well - defined.

4.8.2 Numerical errors

Two numerical errors are worthy of attention here; one is associated with the approximations made in deriving the finite difference equations and the other may arise when they are solved iteratively.

The former source of inaccuracy arises in the process of transforming the partial differential equations into algebraic forms, during which assumptions are made regarding the variation of Φ/C over the control volume. Such assumptions are accurate only when the grid spacing is sufficiently small; thus the stream-wise and cross-stream grid intervals must be systematically reduced until these errors become insignificant, which will be signalled by the insensitivity to further refinement (the solution is then said to be 'grid-independent').

In subsection 4.4 it was mentioned that in solving for the concentration field an iterative procedure is employed, which requires that sufficient iteration 'sweeps' be made to ensure that the solution satisfies the finite-difference

equations to the required degree. In order to assess the degree of completeness of the solution at any stage in the calculation the total residual R_c is calculated: this is defined as follows

$$R_c = \sum_{\text{all nodes}} \left| a_n{}_{i,j} C_{i,j+1,k} + a_s{}_{i,j} C_{i,j-1,k} + a_e{}_{i,j} C_{i+1,j,k} \right. \\ \left. + a_w{}_{i,j} C_{i-1,j,k} + a_u{}_{i,j} C_{i,j,k-1} + S U_{i,j} - (aP - sP)_{i,j} C_{i,j,k} \right| \quad (4.60)$$

The lower the value of R_c the more error free is the solution.

4.9 Closure

A marching or parabolic solution procedure has been presented for plume dispersal calculations which solves numerically the hydrodynamic and energy equations on a two dimensional grid, while solving the pollutant concentration equation on a three dimensional grid that is independent of the hydrodynamic grid system.

Validation of the procedure and presentation of the results are discussed in Chapter 6.

CHAPTER 5

EXPERIMENTAL STUDY

An experimental investigation was carried out with the purpose of validating the present numerical procedure and also complementing existing diffusion measurements.

The experiments were performed in the Atmospheric Wind Tunnel of the Fluid Mechanics Laboratory; Ecole Central de Lyon. The Study included measurements of mean concentrations downstream of a 'point' source where ethane gas was injected into a turbulent boundary layer developed over an aerodynamically 'smooth' surface. Effects of change in surface roughness (smooth to rough) and height of injection on the development of the plume were investigated. Also measured were the mean velocities and the turbulent quantities $\overline{u_1^2}$, $\overline{u_2^2}$, $\overline{u_3^2}$ and $\overline{u_1 u_3}$.

Description of the wind tunnel, ancillary equipment and the procedure employed are given in section 5.1. In section 5.2 the experimental conditions are described and finally certain of the results obtained are presented in section 5.3. However in order to avoid repetition, the main body of the results is presented and discussed in chapter 6 where they are compared with the computer predictions.

5.1 Apparatus and procedure

5.1.1 Wind tunnel

The wind tunnel employed in the present study, shown in figure 5.1 is an open circuit type having a test section

9 m long, 1 m wide and 1.2 m high. The floor of the test section is made from polyster which gives an aerodynamically smooth surface. The angle of inclination of the tunnel ceiling is adjustable in order to regulate the streamwise pressure gradient.

The air flow is produced by a blower mounted at the tunnel entrance and driven by a 35 h.p. variable-speed electric motor. The latter can be regulated to produce mean velocities varying from 2 m/s to 20 m/s with a stability of 1.5%.

In order to increase the thickness and stability of the boundary layer, the latter is tripped at the start of the test section by means of the U-shaped roughness strip shown in figure 5.2.

The measuring probes (which include a Pitot-static tube, hot-wire probe and a sampling tube) are mounted on a motor-driven carriage that is capable of traversing them in the three spatial coordinates. The error of positioning the probes is less than 0.5 mm in the vertical and lateral directions and 5 mm longitudinally.

The tracer gas representing the 'pollutant' is introduced on the vertical symmetry plane of the tunnel 6 m downstream of the test section entrance. The height of the source can be varied from 'ground' level to about 10 cm. A diagram of the injection tube (or source) is shown in figure 5.3.

Two types of surface conditions were used: one was fully-smooth and the other had roughness elements attached commencing 0.5 m downstream of the source location. The roughness elements consisted of square wooden ribs of 3 mm

side, which spanned the width of the tunnel. The ribs were glued to the tunnel floor at 3 cm intervals and extended over a total length of 2.5 metres as shown in figure 5.4.

The motives for the choice of this particular roughness arrangement were ease of manufacture and fitting and the requirement that they should produce the aerodynamic characteristic of a 'fully rough' surface as defined by Schlichting (1968). According to the latter reference, the fully rough condition is obtained when

$$\frac{u_* k_s}{\nu} > 70$$

where k_s is the equivalent sand roughness of the surface. Obedience to this requirement ensures that the longitudinal velocity variation with height is independent of $u_* k_s / \nu$ and this facilitates comparison between experimental and predicted* results. The value of k_s found with the present roughness pattern was 0.024 m which corresponds to $x_o = 0.0008$ m.

*When $u_* k_s / \nu < 70$ the logarithmic law of the wall is dependent on both $u_* k_s / \nu$ and x_o / k_s (note $k_s \propto x_o$) and thus in this case a new law must be devised to incorporate in the numerical procedure.

5.1.2 Measurements of mean velocity and turbulence

(a) Mean velocity: The local stream-wise mean velocity measurement was achieved by means of both a pitot-static tube and hot-wire anemometer. The former had a spherical head with internal and external diameters of 1 and 3 mm respectively, and was connected to a Betz-type micro-manometer which has a precision of about 0.05 mm of water.

The main-stream velocity was monitored by means of a pitot-static probe permanently placed outside the boundary layer.

(b) Turbulent stresses: The hot-wire anemometer was used to measure the velocity fluctuations u_1 and u_3 : in one case u_2 was measured as well. From these measurements turbulent stresses such as $\overline{u_1^2}$, $\overline{u_2^2}$, $\overline{u_3^2}$, $\overline{u_1 u_3}$ etc. could be deduced.

The hot-wire anemometer set-up employed is shown in figure 5.5. The basis of operation is as follows*: the outgoing voltages E_1 and E_2 from the two elements of the cross-wire constant-temperature probe of the anemometer are fed to an analogue circuit that produces two output signals[‡] $f_1(U_1) (\equiv E_1 + \kappa_1 E_2)$ and $f_3(U_3) (\equiv E_1 - \kappa_2 E_2)$; where κ_1 and κ_2 are constants) which are functions only of $\overline{U}_1$ and $\overline{U}_3$ respectively. These signals are then passed through low pass filters which cut out frequencies in excess of 10 KHz in order to reduce noise levels. The filtered signals are

*Details of the types of equipment are given in figure 5.5.

‡Details of the procedure are given by Compte - Bellot and Matheiu (1958).

amplified and then transformed to digital form by an analogue to digital converter; finally the data are stored on the magnetic disc of a Hewlett Packard 2108 computer.

Once the processed $f_1(U_1)$ and $f_3(U_3)$ are stored the calibration characteristics of the probes which are also stored on disc are then employed to obtain U_1 and U_3 . It is then straightforward to calculate numerically $\overline{U}_1$, $\overline{U}_3$, $\overline{u}_1^2$, $\overline{u}_3^2$, $\overline{u_1 u_3}$ etc. as well as higher order correlations and auto-correlations involving u_1 and u_3 , if so desired. Further details on the data acquisition system can be found in Melinand et al (1977).

The acquisition of data was made at a rate* q of 10000 16-bit words/s and each acquisition was performed for a time T of 6 seconds. These values of q and T were chosen so as to be larger than twice the reciprocal of the expected Kolmogoroff time scale and the time scale of the energy-containing eddies respectively as suggested in Bradshaw (1971).

A small proportion of the measurements (mainly for the smooth wall) were made by a different analogue system described by Schon (1974). When comparisons were made between the two set-ups discrepancies of less than 4% were observed which were usually confined to regions of low turbulence intensities, where noise to signal ratios are high.

*The maximum acquisition rate is 120,000 words/second.

(c) Estimation of the friction velocity: The friction velocity u_* was determined by two methods; one was finding the value of u_* that would fit the velocity profile near ground level ($x_3 u_* / \nu < 200$) to the logarithmic law of the wall (equation (4.47)/(4.48)) and the other was by assuming that the shear stress near the ground is approximately constant with height, the value of u_*^2 is then taken equal to the measured $\overline{u_1 u_3}$ correlation closest to ground level. The discrepancy between the two methods was within 6% for measurements of the flow over smooth boundary and within 3% for the case of the rough surface flow measurements. The value of u_* reported here were those obtained by the latter method.

(d) Calibration of hot-wire: Calibration of the hot-wire probe was made by inserting the probe at the centre of the outlet section of a low-turbulence ($u'/U_1 \sim 0.1\%$) calibration tunnel which had the facility of accurately and independently measuring the air velocity by means of a pitot tube as well as heating and controlling the air temperature.

The normal calibration temperature was 20°C but this was varied to assess the sensitivity of the wires to ambient temperature variations. This sensitivity was measured at one velocity and was then assumed to prevail over the full velocity range encountered in the investigation.

5.1.3 Mean temperature measurements

The temperature was measured at a stationary point (2m downstream of the source) in the tunnel by means of a platinum resistance probe having a 3 mm diameter. The probe was connected to a digital voltmeter (DIGTEC 1501) which has

a scale reading precision of 0.01°C .

5.1.4 Concentration measurements

The diffusion measurements were carried out by injecting ethane from a 'point' source into the turbulent boundary layer developed over the floor of the tunnel. Scans were made over a regular lattice of points in planes normal to the ground surface at four downstream locations from the source. At each location a sample was extracted, analysed by means described below and the value of concentrations there recorded.

Ethane was employed as the tracer gas because it has approximately the same density as air (hence buoyancy effects are avoided) and further it is not absorbed by the polyster floor of the tunnel.

The measurement of ethane concentration was made by a 'Beckman' hydrocarbon analyser type 109A. The output of the analyser is a voltage that is directly proportional to the concentration of ethane in parts per million in the sample extracted. The response time of the analyser is of the order of a few seconds. Further details of the principles of the analyser are given by Solal (1972).

The tracer measurements involve two flow circuits, one being for the injection of the ethane and measurement of its flow rate and the other for extracting of the sample and measurements of its concentration.

In the supply circuit pure ethane from bottle containers is circulated through the elements shown in figure 5.6. Two flow measuring devices are employed, namely a rotameter

(which is relatively inaccurate in absolute terms) which is used for monitoring the constancy of the flow rate and a soap-bubble flow meter which is used to accurately measure the rate.

The sample extraction circuit shown in figure 5.7 comprises the sampling tube which is connected by tubing to the extraction pump, from whence it is delivered to the Beckman analyser. The signal from the latter is fed to a Mosley 7100 BM graph recorder.

The injection rate in all cases investigated was maintained at approximately* $0.05 \text{ m}^3/\text{hour}$, which gave an injection velocity of about 0.7 m/s . The rate of sample extraction was set at $0.054 \text{ m}^3/\text{hour}$. Sampling time was 90 s , this value was determined from trials made with sampling intervals of 1, 2.5, 3 and 4 minutes and the time chosen was the lowest that gave average concentrations that are indifferent to the sampling time.

The accuracy of the concentration measurements by the foregoing method was estimated by Solal (1972) to be of the order of 5%.

5.2 Experimental conditions

In all the experiments the tunnel roof was adjusted to give a zero streamwise pressure gradient, the free stream velocity was set at 5.85 m/s ($\pm 1.5\%$) and the flow was neutrally stratified.

*Higher flow rates, which are desirable from the point of view of accuracy of measurements, were not employed for economical considerations.

Hydrodynamic measurements were taken at locations 0, 1, 1.5 and 2.5 m downstream of the source, with an average of 19 measuring points at each location.

A check on the two dimensionality of the flow field was made by measuring the longitudinal velocity $\bar{U}_1$ at different lateral distances. Within experimental error no variation of $\bar{U}_1$ was observed (the lateral scan was restricted to 0.25 m on either side of the tunnel axis). However on measuring the lateral velocity $\bar{U}_2$, it was found that this velocity reached values of up to 2% of the free stream velocity; also the correlation $\overline{u_1 u_2}$ assumed at times values as large as $0.07 u_*^2$. These relatively high values of $\bar{U}_2$ and $\overline{u_1 u_2}$ were observed for the case of the partially rough wall 2.5 m downstream of the source (i.e. 8.5 m from the entrance of the test section), and lower values were measured elsewhere.

For the diffusion experiments two source heights were employed, one being at ground level and the other at a height of 7 cm from the tunnels floor. In the former case experiments were performed with both smooth and partially-rough surfaces, while with the elevated source only the smooth surface case was investigated. Concentration measurements for the ground release were made at the 0.5, 1, 1.5 and 2.5 m downstream locations, while for the elevated release the locations were at 0.5, 1, 1.5 and 2 m downstream. On the average about 90 measuring points were scanned at each downstream plane.

For purpose of assessing reproducibility measurements were made at selected locations at different times under

nominally the same experimental condition and was found that the results could be reproduced to within 7%.

5.3 Results

5.3.1 Flow field

The majority of the results are presented and discussed in chapter 6: here only some of the results for the flow over the smooth surface are presented and compared to similar experiments made by Klebanoff (1954).

Figure 5.8 shows the profiles of velocity and shear stress, at $x_1 = 0$ where x_1 is now the longitudinal distance measured from the source, non-dimensionalised by $U_{1\infty}$ and u_*^2 respectively and plotted against x_3/δ (δ is defined here as the height where $\bar{U}_1 \approx 0.995 U_{1\infty}$). The results are compared to those made by Klebanoff (1954)). Though slightly higher, the velocities of the present study compare well with Klebanoff's. Agreement of the shear stress is considered to be good in the near wall region however with larger discrepancies from Klebanoff's measurements observed further away from the wall.

The normal stresses $\bar{u}_1^2$ and $\bar{u}_3^2$ are shown plotted at different downstream locations in figure 5.9. The agreement with Klebanoff's results seems to be closer the larger the downstream distance .

5.3.2 Concentration

The concentration measurements are given in tabular form in Tables 5.1, 5.2 and 5.3 for the three cases of ground release with a smooth tunnel surface, ground release

* For values of u_* and δ See fig 6.3.

with a step change in surface roughness and elevated release over a smooth surface respectively. Some of these data are shown plotted in figures* 5.10 - 5.20.

One important feature shown by these results is that the centre plane of the plume (defined as the plane about which the plume is 'symmetric') veers away from the tunnel symmetry plane as the plume spreads downstream. This behaviour can be attributed to the finite lateral velocity mentioned earlier. A similar behaviour was observed in Solal's (1974) data, however the present results show much less skewing of the plume about its axis than that found in Solal's experiments.

The amount of deviation of the plume axis from that of the tunnel is shown plotted in figure 5.21 against x_1 for the three experiments carried out.[‡]

Further details about the concentration data are given in chapter 6.

5.4 Closure

An experimental study was carried out to investigate the dispersal of a point source in a turbulent boundary layer. Measurements of concentration fields were made to assess effects of source height and change of surface roughness on the dispersal.

*The negative axis in these figures refers to the left section of the plume when viewed in the upstream direction.

[‡]Henceforth all diagrams plotted involving concentration profiles will have the plume axis shifted to the tunnel's axis.

The flow field was also investigated and measurements were taken of mean and turbulent velocities for a continuously smooth wall and one where a change in surface roughness occurred. Results are reported for the former case and compared to those of Klebanoff.

CHAPTER 6

PRESENTATION AND DISCUSSION OF RESULTS

In this chapter the results obtained from the numerical calculations and the experiments carried out in the present study are presented, compared and discussed.

The presentation commences in Section 6.1 in which an account is given of preliminary studies carried out to validate the numerical solution procedure and also to establish the grid density required to obtain acceptable accuracy. The remaining part of the chapter is divided into two main sections, these being Section 6.2 which deals with the hydrodynamic and temperature* fields; and Section 6.3 which is devoted to measurements and prediction of the concentration field.

6.1 Preliminary Validation studies

Preliminary studies were undertaken with the purpose of validating the numerical procedure in the absence of uncertainties associated with the physical modelling. To achieve this all transport properties (e.g. diffusivities) were prescribed and predictions were made from selected cases for which analytical solutions existed.

*The temperature field is of interest here only when inflicting buoyancy effects on the flow.

The initial test case for the hydrodynamic calculation is that of a laminar boundary layer flow over a smooth flat plate in the circumstance of zero streamwise pressure gradient. The starting condition for the solution was a uniform-velocity flow parallel to the plate. The calculations were carried out with 14 grid lines in the vertical direction and a forward step size equal to 0.1δ ; these specifications being found by trial and error yield results that were insensitive to further grid refinement. The predicted values of $\bar{U}_1$, $\bar{U}_3$, δ and τ were found to be in perfect agreement (maximum error less than about 0.5%) with the series solution obtained by Blasius, as quoted by Goldstein (1965).

The initial test case for the concentration calculation is that of a point source emitted into a homogeneous field having uniform prescribed velocities and diffusivities, with K_2 not necessarily equal to K_3 . The predicted concentrations were compared with the analytical solution quoted in Hinze (1975), and revealed maximum errors of less than 0.5%. This level of agreement was achieved with a 12 x 12 grid in the cross-stream plane* and a forward step size of 5% of the plume thickness.

Exploratory calculations were also performed for the general case, in which all equations were solved, (including those for the turbulent fluxes), in order to establish a

*Symmetry allowed the calculations to be confined to one quarter of the plume cross section.

grid specification which would yield solutions insensitive to refinement. It was found that for circumstances corresponding to wind tunnel experiments 21 cross-stream nodes sufficed for the hydrodynamic calculations and a 16×14 grid was adequate for the concentration field. For atmospheric dispersal calculations the only change required was to increase the hydrodynamic grid nodes to 23. The forward step employed in all calculations was 0.025 the plume size.

6.2 Hydrodynamic and temperature fields

This section is divided into two parts, one dealing with flows under neutral conditions and the other with thermally-stratified conditions. In the former case measurements of laboratory flows are used to validate the calculation procedure, since these are generally made under controlled conditions and have known uncertainty limits, whereas neither of these comments applies to measurements in the atmosphere. For the stratified cases, however, reference will be made to atmospheric flows, the main reason being the absence of laboratory data for significant levels of stratification. There is of course the additional incentive of the direct relevance to atmospheric dispersal.

6.2.1 Hydrodynamic characteristics of neutral flows

(a) Continuously-smooth surface: The data used for comparison here are from the classical experiment of Klebanoff (1954). In Figure 6.1 the predicted mean stream-wise velocity non-dimensionalised by the free stream velocity $U_{1\infty}$ is shown

plotted against x_3/δ . Also shown in Figure 6.1 are normalised profiles of the shear stress $\overline{u_1 u_3}$. Agreement of the present predictions with Klebanoff's* data is considered to be fairly good. Similar agreement is observed for the normalised normal stresses $\sqrt{\overline{u_1^2}}/u_*$, $\sqrt{\overline{u_2^2}}/u_*$ and $\sqrt{\overline{u_3^2}}/u_*$ as shown in Figure 6.2. For the conditions of these comparisons the numerically predicted value of the ground shear stress was found to be 3.5% greater than Klebanoff's measurement. The level of agreement (between the present predictions and Klebanoff's results) obtained here was found to be similar to that obtained by Launder et al (1975) who solved the full partial differential equation for Reynolds stresses. This demonstrates the adequacy of the simplified algebraic stress model to simulate the present flow situation.

(b) Surface with a step change in roughness: The experiments simulated here are those carried out in the present investigation, details of which were given in Chapter 5.

The variations of the shear velocity and boundary layer thickness are presented in Figure 6.3, from which it is seen that at the point where the rough region begins ($x_1 = 0.5$ m) the predicted u_* rises sharply and then rapidly decays to a level which is higher than that for the smooth wall upstream. Unfortunately no measurements were taken in this region but the observed behaviour of u_* is plausible;

*The Reynold number Re_δ at the location at which results were presented for both Klebanoff's results and the present prediction was in the vicinity of 75000.

for as the upstream fluid encounters the roughness the near-wall fluid undergoes a sudden deceleration, giving rise to steep velocity gradients and hence the observed high values of u_* . As the surface flow effects propagate through the velocity gradients reduce towards the near-equilibrium values appropriate to the new surface condition.

Further evidence of the above-described phenomena can be seen in the response of the boundary layer thickness δ to the change in the surface roughness. As demonstrated in Figure 6.3, the rate of increase of δ is augmented when the flow reaches the rough region. This is a consequence of two factors; first, the deceleration of the flow in the streamwise direction, necessarily causes the flow to be displaced upwards and secondly the augmentation of turbulence produced by the rough wall promotes mixing of the flow in the free stream with that in the boundary layer*.

It should be stated here that some uncertainty exists in the use of the logarithmic law (4.47) in the application of the prediction method to the vicinity of a step change in surface roughness, since the law was essentially derived for conditions in which the flow has reached a developed, near-equilibrium state (Townsend (1976)). However unless precise prediction is required in this region (in which case the present procedure might prove inaccurate) the logarithmic law seems to perform adequately as implied by

*The effect of this comes in downstream of the start of the rough region when the 'internal layer' (defined later) has grown sufficiently.

the good agreement between predicted and experimental values of u_* further downstream.

The development of the velocity profile with x_1 is shown in Figure 6.4 where profiles are shown at different downstream locations. It is clear from this figure that the effects of the roughness change propagate through the boundary layer as it flows downstream, as is demonstrated by the values of diminishing $U_1/U_{1\infty}$ in the affected regions. Agreement between experiments and numerical predictions is within 5%.

Profiles of the Reynolds stress components downstream of the roughness change are shown in Figures 6.5 to 6.10. The figures show comparisons between predicted and experimental results, for the normalised shear stress in Figures 6.5 to 6.7 and normalised, normal stresses in Figures 6.8 to 6.10, at various x_1 locations. In general agreement between experiment and prediction displayed for $\overline{u_1 u_3}$, $\overline{u_1^2}$ and $\overline{u_3^2}$ is quite good.

Due to lack of time available for the experimental program $\overline{u_2^2}$ was measured solely at $x_1 = 2.5$ m; agreement between the measured and predicted values of $\sqrt{\overline{u_2^2}}/u_*$ shown in Figure 6.10 is considered to be only moderate. No exact reason can be given to the observed disparity; however it ought to be mentioned that the constants, which appear in the near wall correction terms ϕ_{ijw1} and ϕ_{ijw2} , were set so as to give the observed near wall values of the calculated stresses, hence if the measured values (of $\overline{u_2^2}/u_*^2$) are correct the value of these constants must be reviewed.

In each of the Figures (6.5) to (6.10) two distinct regions can be identified, one being the layer near the surface that has been affected by the extra generation caused by the increased roughness, this is sometimes referred to as the 'internal layer'. The second region is the remainder of the boundary layer where the flow field is relatively undisturbed by the new boundary conditions and the stresses there are comparable in value to the approach conditions (i.e. of the smooth wall). That the latter statement is correct can be shown by normalising the Reynolds stresses of a location downstream of the change in roughness by a value of u_* , pertaining to the smooth wall*, and then comparing them with their equivalents for smooth-wall flow. Such comparisons are shown in Figure 6.11 for $\overline{u_1 u_3}$ and Figure 6.12 for $\overline{u_3^2}$ and $\overline{u_1^2}$, both of which contain profiles for $x_1 = 0.45$ m (which is in the smooth region) and $x_1 = 1$ m. It is seen from Figure 6.11 and Figure 6.12 that profiles on the smooth and rough sections are approximately equivalent for value of $x_3/\delta < 0.32$ while close to the wall larger values are observed for the flow over the rougher region; this suggests that the internal layer at $x_1 = 1$ m is approximately equal to 0.32δ .

6.2.2 Buoyant flows

The majority of data on buoyant or stratified flows

*The value of u_* is taken as that at $x_1 = 0.45$ m.

are analysed in terms of the similarity theory of Monin and Obukhov (see Monin and Yaglom (1977)); it thus seems appropriate at this stage to give a brief account of this theory and its validity.

According to the similarity theory of Monin and Obukhov in a horizontally homogeneous surface layer all appropriately normalised and averaged variables are universal functions of x_3/L only; provided that the height considered is sufficiently larger than x_0 .

The validation of similarity hypothesis was one of the main objectives of investigations carried out both on atmospheric data (e.g. Wyngard et al (1971), Businger et al (1971)) and on wind tunnel experiments (e.g. Schon (1974), Arya and Plate (1971)). The results from the former studies have indicated that within the observed scatter similarity theory was found to be reasonably applicable in the surface layer. However slight deviation of the data from the theory was observed by some workers (e.g. Wyngard (1973)) and this, together with the considerable scatter led them to question the possibility of parameters other than x_3/L being influential such as the boundary layer thickness.

In an effort to procure better control over experimental conditions and facilitate measurements Arya and Plate (1971) conducted experiments on stably-stratified flows in a wind tunnel. Though there is a trend from their measurements to support the similarity theory nonetheless the data do reveal some dependence* of normalised variables such as

*The majority of Arya and Plata's data were made outside the constant stress/flux region (which would correspond to the surface layer in the atmosphere) and hence their results /contd.

$\sqrt{\bar{u}_1^2}/u_*$ (for the same x_3/L variables at different x_3/δ have different values) moreover a great deal of scatter is observed. This anomaly in Arya and Plate's results was also displayed in Schön's (1975) experimental data for unstable stratified flows.

We now start the presentation of results from the present calculation and we commence with unstably stratified flows.

(a) Unstable stratification: Figure 6.13 shows predictions and the empirical fit to experimental data under atmospheric conditions, given by Businger et al (1971) for the normalised velocity gradient $\phi_m (\equiv \bar{u}_{1,3} x_3 / u_*)$. The empirical equation is:

$$\phi_m = (1 - 15x_3/L)^{-0.25} \quad (6.1)$$

No details on the conditions (e.g. δ , temperature gradient across the boundary layer, geostrophic wind speed ... etc.) under which the experiments were performed was quoted; in the calculation the results presented are at a downstream location where the boundary layer thickness was about 950 m, the difference in the potential temperature across the layer was 3°K and the free stream velocity was 6 m/s. These values would yield an overall Richardson Rf_δ number defined as

could not with certainty prove or disprove the similarity hypothesis. Further, in order to reach high stratification the mean velocity was reduced to the extent that their data could be prone to low Reynolds number effects.

$$Rf_{\delta} = g\delta \frac{\Delta\theta_m}{\theta_m} / U_{1\infty}^2 \quad (6.2)$$

of 2.68.

It is interesting to note the effect of the turbulence modelling constant $c_{\epsilon 3}$ on the prediction* of ϕ_m ; from Figure 6.13 it is seen that as $c_{\epsilon 3}$ increases ϕ_m also increases; this result is to be expected since augmentation of $c_{\epsilon 3}$, will in unstable flows, be accompanied by an augmentation of the dissipation rate and hence a decrease in the turbulence intensity and reduction in the latter would in turn lower the velocity gradients. It is obvious from Figure 6.13 that with the present model elimination of the extra buoyant term in the ϵ equation by setting $c_{\epsilon 3}$ to zero, as suggested by Gibson and Launder (1975) would produce unacceptably low values of ϕ_m .

To assess the dependence of the variation of ϕ_m predicted by the present model on parameters other than x_3/L , three different levels of overall Richardson numbers were imposed. The results, for Rf_{δ} ranging from 1.75 to 4.53, shown in Figure 6.14, reveal that a change of about 160% in Rf_{δ} brings about a variation of up to 25% in ϕ_m at a given value of x_3/L . Whether such a behaviour is correct cannot be resolved, at present with certainty due to the uncertainties in the experimental data mentioned earlier, hence it must remain an open question for the present. All further results shown pertinent to unstable

*It is to be noted that the value of $c_{\epsilon 3}$ (=1.55) used in this investigation was obtained by trial and error to achieve best agreement with equation 6.1.

stratification are presented under conditions where the overall Richardson number is 2.68.

Figure 6.15 illustrates the variation of $\bar{u}_3^2/u_*^2$ with x_3/L . The same trend is exhibited by both predictions and the experimental results quoted in Wyngard et al (1971), namely an increase in u_3^2/u_*^2 with $-x_3/L$, but the calculations seem to underestimate the level of the vertical velocity fluctuations by about 10%. Gibson and Launder (1978) found a similar discrepancy between their predicted results and those of Wyngard et al (1971), which they attributed to an erroneously low measured ground shear stress, which would of course displace the normalised data upwards.

Prediction of the cross-stream variation of the dissipation rate ϵ , non-dimensionalised by the mechanical production rate of k at ground level, u_*^3/kx_3 , is found to be in good agreement with the experimental data given by Wyngard and Cote (1971) as demonstrated in Figure 6.16. This level of agreement, it should be mentioned, should not be taken as strong evidence of the ability of the present procedure to predict ϵ since the assumptions underlying the measurements grossly over-simplify the real situation.

The variation of the normalised temperature gradient $\phi_T (\equiv \overline{\theta}_{,3} x_3 / T_*)$ with $-x_3/L$ is shown in Figure 6.17. The predictions are found to be of a maximum of about 10% higher* than the experimental data at low values of $-x_3/L$, while at larger $-x_3/L$ much better agreement is observed.

(b) Stable stratification: Unlike unstable stratification in stably-stratified flows energy is extracted from the turbulent motions by the action of buoyancy forces. As the level of stability increases there is a critical stage reached where the turbulence ceases** to exist and eventually the flow reverts to a laminar state. The Richardson number at which this phenomenon occurs is known as the 'critical Richardson number' and was estimated by Arya (1972) to be in the range 0.15 to 0.25 in the surface layer.

*If Gibson and Launder's (1978) suggestion of an under-estimation of the measured shear stress is correct and if the heat fluxes were measured correctly, these factors together would imply higher values for T_* which in turn would produce lower normalised temperature gradients.

**Arya (1972) explains that the likely reason for this phenomenon is not only because of actual drain of turbulence energy but also suppression of the mechanism by which mean flow energy is being converted into turbulence.

Because of the relatively small value of the critical Richardson number, it was originally thought that the present predictions for this case would be less sensitive* to the value of $c_{\epsilon 3}$ than in the unstable case where the upper limit on Richardson number could theoretically reach infinity. This however proved to be false and the value $c_{\epsilon 3}$ was found to appreciably influence the results under stable conditions. Moreover the value of 1.55 chosen for this constant on the basis of the unstable-stratification behaviour yielded predictions of non-dimensionalised velocity gradients which were as much as 100% in error for the stable case.

Further explorations revealed that the best agreement for stable stratification is obtained with a value of $c_{\epsilon 3}$ of zero i.e. by entirely suppressing the buoyant term in the dissipation equation: this is shown in the ϕ_m comparisons in Figure 6.18. This value of $c_{\epsilon 3}$ has been used in all subsequent calculations under stably stratified conditions.

*A smaller Richardson number implies a smaller buoyant term (relative to, say, shear production) in the dissipation equation and thus $c_{\epsilon 3}$ which multiplies the buoyant term will be less influential.

It would have of course been desirable to obtain a model with a universal set of true constants, but because the modelling of the dissipation* equation is at present based mainly on intuition, with the assistance of dimensional analysis and requirements of tensor invariance, there is little prospect of achieving this in the immediate future.

6.3 Concentration field

This section is divided into two parts, one dealing with wind tunnel dispersal and another with atmospheric diffusion. Greater emphasis is placed on the former because of the more reliable and well-defined conditions in wind tunnel experiments form a better testing ground than the atmospheric measurements; also results from wind-tunnel experiments tend to be more detailed.

6.3.1 Wind tunnel dispersal

(a) Line source ground release: The experimental data used for comparison with the present numerical approach for this situation are those of Poreh and Cermac (1964). These authors measured the dispersion of ammonia gas into a turbulent boundary layer from a steady line source on the wall oriented normal to the flow.

Poreh and Cermac found that, provided the plume is 'well-embedded' in the boundary layer but has dimensions much larger than the laminar sublayer thickness then $U_1 C_m / Q'$ (where Q' is the source strength/length) and the

*The reason for 'blaming' the dissipation equation is that, by employing a prescribed length scale and assuming energy equilibrium (and hence by-passing the need for the dissipation equation) Gibson and Launder (1978) obtained fairly
/contd.

half width of the plume λ_3 defined by:

$$\bar{C}(x_1, \lambda_3) = 0.5C_m \quad (6.3)$$

are independent of the free stream velocity and the initial boundary layer thickness δ_i . This behaviour they found was restricted to what Poreh and Cermac call the 'intermediate region' which extends to a downstream distance of about $18\delta_i$ from the line source (the location of the beginning of this region was not stated). The following relations were given by the forementioned authors (in c.g.s. units) as a fit to their experimental data in the intermediate region:

$$U_{1\infty}C_m/Q' = 26.2x_1^{-0.9} \quad (6.4)$$

$$\lambda_3 = 0.076x_1^{0.8} \quad (6.5)$$

The present numerical predictions are compared to the Poreh and Cermac results in Figure 6.19, where λ_3 and $U_{1\infty}C_m/Q'$ are shown plotted against x_1 . This diagram reveals that the predictions follow the empirical relation (6.5) up to values of $x_1/\delta_i < 18$ i.e. to the end of the intermediate region; beyond this, predictions deviate as expected from the empirical relations. For example the predicted rate of spread is smaller and in better agreement with the experimental data.

good results with a similar algebraic model. (Gibson and Launder's procedure is accurate only when the situation considered is near equilibrium and the length scale is known.)

The reason for the reduction of the rate of increase of λ_3 , for values of $x_1 > 18\delta_1$ is that at such downstream locations the plume starts to traverse the edge of the boundary layer; since outside the boundary layer diffusion is performed mainly by molecular action further expansion of the plume becomes limited by the increase in δ .

The predictions also revealed that the values of λ_3 and $U_{1\infty}C_m/Q'$ in the intermediate region, were in agreement with the experiments, independent of the initial boundary layer thickness δ_1 as is shown in Figure 6.19. Figure 6.20 shows that in the same region λ_3 and $U_{1\infty}C_m/Q'$ are also insensitive to variations in $U_{1\infty}$; at larger downstream distances however the plume spread was found to decrease with increase in velocity; this is thought to be due to the smaller value of δ accompanying higher velocities.

The initial insensitivity of the dispersal to the free-stream velocity could be explained by noting that as the latter increases the time available for dispersal ($\approx x_1/\bar{U}_1$) decreases, while the turbulence level simultaneously increases* and these effects apparently counterbalance each other.

Poreh and Cermac (1964) also reported that in the intermediate zone the local time-mean concentration normalised with its maximum i.e. $\bar{C}/C_m$ is insensitive to parameters other than x_3/λ_3 . However, by similarly normalising the

*For Reynolds numbers based on x_1 (i.e. $U_{1\infty}x_1/\nu$) lying between 5×10^5 and 10^7 Schlichting (1968) gives $u_*^2 = U_{1\infty}^2 0.0128 Re_\delta^{-0.2}$ i.e. u_* is a weak function of Re_δ while being almost directly proportional to $U_{1\infty}$ (note that close to the ground $k \approx 4u_*^2$).

governing differential conservation equation of the mean concentration it is shown in Appendix E1 that exact 'similarity' is not to be expected.

Figure 6.21 shows predicted and measured profiles of $\bar{C}/C_m$ vs x_3/λ_3 at various streamwise stations. It is evident that the predicted profiles (which lie within the experimental scatter) are not exactly independent of x_1 .

(b) Elevated line source: Predictions for an elevated line source were made to simulate the experiments of Paranthoen and Trinite (1973) where an electrical wire dissipating heat at a rate of 3.25 w/cm was placed parallel to the wall and perpendicular to the main flow. The Reynolds number of the flow Re_δ at the source was 17100; the ratio of height of release to boundary layer thickness was 0.5.

Predictions and measurements of the vertical temperature deficit $\Delta\bar{\theta}$ (defined as the difference in temperature between a point in the plume and ambient temperature) distributions are presented for several downstream locations in Figure 6.22. From this, it is apparent that the location of maximum temperature is slowly shifting towards the wall as the plume moves downstream. This shift is a consequence of two factors:

- (i) Lower* velocities exist near the wall.
- (ii) At the outer boundary of the plume, temperatures are reduced due to entrainment of cold fluid while at the wall the heat is preserved because it is, in principle, adiabatic.

*For a specified flux, the concentration is inversely proportional to the mean velocity i.e. the smaller the velocity the higher the concentration.

It is evident that the numerical predictions slightly over-estimate both the temperature level and the plume spread. There seems to be a contradiction in this result because, in order for overall conservation of energy to prevail, an increase in spread must be accompanied by a decrease in temperature level (assuming of course that predicted and experimental velocity profiles are the same). The implication is therefore that there is a heat loss* to the wall in the experiment as is indeed suggested by existence of temperature gradients there. Despite the discrepancies, the overall agreement may be considered to be moderately good.

(c) Point source, ground release

Smooth wall: The variation of lateral and vertical spreads λ_2 (defined by $\bar{C}(x_1, \lambda_2, 0) = 0.5C_m$) and λ_3 respectively with x_1 for a point source released into a turbulent boundary layer is shown in Figure 6.23 which contains experimental results from Malhotra and Cermac (1964), Solal (1972) and the present experiments. Predictions were made to simulate each of these experiments (i.e. by employing where possible the same values of δ , $U_{1\infty}$... etc. and initial conditions reported in the experiments) and are also shown on Figure 6.23. The following points emerge from the comparison:

- (i) The vertical spread λ_3 seems to be insensitive to variations in velocity (the predictions suggest a slightly higher spread for lower velocities) and to initial boundary

*In the numerical procedure the streamwise energy flux is monitored at every downstream location and the energy was found to be conserved to within 0.5% of the initial energy flux.

layer thickness δ_1 (the present experiments had an initial boundary layer thickness 1.4 times that of Solal).

(ii) The values of λ_3 from the different experiments exhibit relatively good agreement among themselves. The predictions on the average lie about 8% below the data.

(iii) Larger scatter between results of different experiments are observed in the values of λ_2 than in λ_3 , with the present data and those of Solal (1972) showing lower values of λ_2 than those of Malhotra and Cermac.

(iv) Both predictions and experiment indicate that the lateral spread λ_2 is also relatively insensitive to the level of free stream velocity (a slightly higher increase in spread with decrease in velocity is suggested by the predictions), but the calculated effect of initial boundary layer thickness on λ_2 is more marked, the tendency being for it to increase with δ .

The result that λ_2 is slightly dependent on δ while λ_3 is independent* may be plausibly explained by reference to the behaviour of the Reynolds stresses u'_2/u_* and u'_3/u_* (in Figure 6.2) which are responsible for the lateral and vertical spreads respectively, as is implied by equations (3.118) and (3.119). The latter figure shows that for values of x_3/δ up to about 0.3, u'_3/u_* is approximately constant while u'_2/u_* has decreased to about 80% of its near-wall value. Thus at a fixed location x_3 within the fore-mentioned region no marked difference in the value of u'_3/u_*

*At least for the regions examined. It is of course expected that when the plume reaches the edge of the boundary layer the rate of increase of λ_3 will fall, as in the case of the line source.

would exist between a 'thick' and thin layer (and hence no effect on vertical diffusion), whereas u_2'/u_* would be larger for the thick boundary layer, and hence would lead to a larger value of λ_2 .

The streamwise variations of the maximum concentration level given by the forementioned experiments and predictions are shown in Figure 6.24. As expected, cases exhibiting higher spreads in Figure 6.23 show lower maximum concentration levels. Agreement between different experiments* and predictions is satisfactory.

The concentration profiles in the lateral direction, plotted in Figure 6.25 as $\bar{C}/C_m$ versus x_2/λ_2 were found in the present experiment as in that of Malhotra and Cermac (1964) to be of Gaussian form which, as illustrated in the same figure, is in perfect agreement with the numerical predictions.

Due to vertical inhomogeneity in both the mean velocities and the turbulent stresses, the concentration profiles in the vertical direction, when plotted as $\bar{C}/C_m$ versus x_3/λ_3 , deviate from a Gaussian distribution. The present measurements shown in Figure 6.26 for the symmetry plane $x_2 = 0$ are fitted well by a profile of the form

$$\bar{C}/C_m = \exp\{-0.693(x_3/\lambda_3)^b\} \quad (6.6)$$

where $b = 1.55$. The present predictions which are also plotted suggest the same form but a different value of $b = 1.4$,

*The value of Q employed to estimate $C U_{1\infty}/Q$ in Malhotra and Cermac (1964) data was 3.8 m.g/s which was reported in Malhotra (1962).

which value happens to be in exact agreement with that found by Malhotra and Cermac (1964) .

Within the ranges of $U_{1\infty}$ and δ_i investigated the shapes of the profiles were found to be independent of both $U_{1\infty}$ and δ_i .

Step change in surface roughness: The effects of a step change in surface roughness on λ_2 and λ_3 are shown in Figure 6.27. It is clear from this figure that on encountering the rough wall (at $x_1 = 0.5$ m) the plume tends to spread at a higher rate than that over the smooth surface. It is interesting to observe that the measured and predicted effects of the rough wall on the ratio λ_2/λ_3 show a reduction* in this over the smooth-wall level.[‡] However, the measurements indicate that λ_2 is approximately equal to λ_3 , the predictions suggest a larger value for λ_2 . The equality of λ_2 and λ_3 suggested by the experiments cannot be easily explained especially if account is taken that the measured values of $\bar{u}_2^2$ are larger than those of $\bar{u}_3^2$ (Figure 6.10); however there does seem to be the tendency in the wind tunnel employed in the present experiments for the lateral spread to be curbed.

Despite the above-mentioned differences the disparity between experiments and predictions of λ_2 and λ_3 is less than 10%, while as Figure 6.28 shows, a much better agreement is obtained for the streamwise variation of maximum

*This is probably the result of the reduction of $\bar{u}_3^2/\bar{u}_2^2$ (compared to the smooth surface) over the rough surface as implied in Figure 6.10.

[‡]For example according to the predictions at $x_1 = 2$ m these rates are equal to 1.52 and 1.16 on the smooth and rough surfaces respectively.

concentration.

Like the smooth wall case, the lateral concentration profiles are found, to be Gaussian, as indicated in Figure 6.29. The vertical variation shown in Figure 6.30 follows equation (6.6); however the exponent is found to be 2.2 to fit the experimental data and between 2 and 2.2 to agree with the predictions.

Elevated point source: The last laboratory flow investigated is the elevated point source. The measurements that are considered here are those of the present experiments and of Davar (1961). Details on the former experimental conditions are given in Chapter 5. In Davar's experiments the pollutant employed was ammonia gas which has a specific gravity of 0.6 that of air, the gas was injected at a height of 0.0254 m with a flow rate maintained at approximately 5.83 cm³/s. The boundary layer thickness at the point of injection was 0.076 cm and the free stream velocity was about 1.82 m/s.

Vertical concentration profiles from the present experiments and the corresponding numerical simulations are plotted in Figures 6.31 to 6.34 at different downstream locations. The agreement between the predictions represented by the solid lines and the data are found to be quite good in respect of both the amount of spread and the concentration level.

It is interesting to observe the effect of employing the turbulence length scale $k^{3/2}/\epsilon$ in place of the currently-preferred concentration-field length scale in the model equation for $\overline{u_3 c}$ (see Section (3.34)). Predictions made with

the former version hereafter referred to as 'model 1' while the preferred version will be called 'model 2' are also shown in Figures 6.31, 6.32 and 6.34 as dashed lines. It is evident that the initial plume spread, is greatly exaggerated but further downstream the disparity between model 1 and experiment diminishes. This result is expected, since near the source location the scales of the concentration fluctuations are small compared to those of the hydrodynamic field and hence a smaller part of the energy spectrum (roughly the part corresponding to motions having scales comparable to the size of the plume) is correlated with the concentration field, than is implied by model 1. Further downstream the plume dimensions more closely approach those of the flow field and this effect is reduced, thereby resulting in better performance of model 1.

Figure 6.35 shows the lateral spreads. Again agreement between model 2 and the present measurements is good while model 1 produces an excessively large spreading rate.

The predicted streamwise trajectories of the plume parameters λ' , λ'_2 and λ_3 where λ' and λ'_2 are defined respectively as

$$\bar{C}(x_1, 0, \lambda') = C_m$$

$$\bar{C}(x_1, \lambda'_2, \lambda') = 0.5C_m$$

are shown in Figure 6.36 for the conditions of Davar's (1961) experiment together with his data, while Figure 6.37 compares the

values of the maximum concentrations. In general agreement is reasonably good, the mean discrepancy being about 6% and 12% for the spreading rate and maximum concentration respectively.

6.3.2 Atmospheric dispersal

The objectives of the predictions carried out here were to produce correlations of the form suggested by Pasquill (1961) for atmospheric diffusion calculations and to compare the results with those of Pasquill. These correlations relate the lateral and vertical spreads with downstream distance for different stability categories. The stability categories vary from 'A' to 'F', with A denoting a highly unstable condition and F a highly-stable atmosphere (D being neutral). Recently these categories have been quantified by Smith (Pasquill (1974)) in terms of the level of surface heat flux, the surface roughness height and the wind velocity at 10 m height. Smith's specifications were employed here to define the stability categories in the numerical simulations.

The calculation procedure was applied to simulate four different stability conditions for a ground level 'point source' release. The running conditions for the cases considered are displayed in table 6.1. With the velocities predicted at $x_3 = 10$ m these cases correspond to categories D-E, E, B-C and B (D-E and B-C refer to a stability condition lying between D and E and B and C respectively). In all cases the initial temperature

profile was assumed uniform, the flow was then allowed to develop for a distance of 5000 m under the specified condition of Table 6.1 before introducing the plume source.

Figure 6.38 shows Pasquill's (1961) correlations for the vertical spread h which is defined as the height where the concentration falls to 10% of the maximum value. This figure demonstrates that the present predictions which are shown as points, agree fairly well with the Pasquill curves for all categories investigated, up to values of x_1 of about 6000 m. Further downstream the spreading rate is underpredicted (especially for the highly-unstable categories). The reason is that at this distance the plume encounters the outer edge of the boundary layer and the subsequent spreading rate is dictated by the expansion rate of the boundary layer, which is small. It would have been possible to avoid this by specifying a larger initial boundary layer thickness; however the Pasquill curves tend to be unreliable at large downstream distance and therefore no further effort was made to obtain better agreement.

It is worthwhile at this stage to note the significance and effect of the correlation $\overline{c\theta}$ on the dispersal. This term appears (multiplied by β_p) in equation (3.19) for $\overline{u_1 c}$ as a destruction/production term (depending on the sign of $\overline{u_1 c}$ and $\overline{c\theta}$). Initially in the present study no physical reason could be given for the existence of a correlation between c and θ and because of lack of data about this it was set to zero. However on further consideration it was

found that a correlation could exist for the following reason; temperature fluctuations appear in the equation for u_i (and hence in the equation for $\overline{u_i c}$) as a consequence of density fluctuations and because the latter is closely associated with the concentration C , a finite value for $\overline{c\theta}$ becomes plausible; possibly a more convincing argument is that the production $P_{c\theta}$ term in the transport equation for $\overline{c\theta}$ has the form:

$$P_{c\theta} = -(\overline{u_j c} \frac{\partial \overline{\theta}}{\partial x_j} + \overline{u_j \theta} \frac{\partial \overline{C}}{\partial x_j})$$

which could be finite (even when $\overline{c\theta}$ is zero) in the presence of gradients in both mean temperature and concentrations.

Unfortunately the absence of experimental data for this correlation hinders determination of the value of the related constant a' in the modelled equation (3.94) for $\overline{c\theta}$ and the only obvious way of estimating it is to choose a value for it that will adequately reproduce one of the Pasquill curves: the B category curve was chosen here for this purpose.

Figure 6.38 shows the results of attempts to simulate categories B and B-C with $\overline{c\theta}$ set to zero. We can see from this figure that inclusion of $\overline{c\theta}$ in the model, increases dramatically the value of h for a specified condition. Under stable circumstances however, $\overline{c\theta}$ is expected to act as a destruction* term of $\overline{u_j c}$ and hence it would tend to

*According to the present model $\overline{c\theta}$ will be positive whenever $\overline{\theta}_j$ and $\overline{C}_j$ have the same sign and is negative otherwise.

reduce the dispersal rate (this case is not shown in Figure 6.38).

The Pasquill correlations for the lateral spread, represented by σ_2 are shown in Figure 6.39 together with the present predictions. It is evident that much smaller values for σ_2 are predicted than are suggested by Pasquill. This result was to be expected since the present calculations currently take no account of changes in mean wind* direction, the values of which are contained in Pasquill curves and tend to increase the apparent rate of spread. Some recommendations about how this effect might be simulated are given in Appendix B1.

6.4 Closure

The conclusion from this chapter may be summarised as follows:-

- (i) The numerical procedure and turbulence model seem capable of predicting adequately the mean velocities and turbulence quantities in boundary layer flows over smooth surfaces and situations where a change in surface roughness occurs.
- (ii) In unstably-stratified flows the proposed model seems to give moderately good agreement with atmospheric data; however some deviation from the Monin-Obukhov similarity theory is observed. Under stable conditions the 'constant'

*What is meant by mean wind here are velocities having time scales longer than the averaging time (see Chapter 2).

$c_{\epsilon 3}$ appearing in the dissipation equation must be set to zero (instead of 1.55 as in the unstable case) to procure adequate agreement with the measured normalised velocity gradients.

(iii) Predictions of the concentration fields in neutral wind tunnel flows over smooth surfaces for both ground and elevated point/line sources are in quite satisfactory agreement with experiments.

(iv) In the case of dispersal over surfaces with a step change in surface roughness, although both experiments and predictions indicate a decrease in λ_2/λ_3 over the rough region, the measurements suggest a value of unity for this ratio while the calculations give an average value of about 1.16. However the resultant inaccuracies in the predictions of λ_2 and λ_3 are less than 10%.

(v) The present predictions of the vertical spread in atmospheric dispersal is in good agreement with Pasquill's (1961) correlations for different stability conditions. The predictions however underestimates the lateral spread; the reason for this underestimation is attributed to the lack of allowance in the model for variation in mean wind direction.

As a final comment, for these calculations the computer code used requires about 220 seconds on a CDC 6500 computer to cover a downstream distance of 20 km while occupying a core of less than 25 kilowords. These requirements seem relatively modest in relation to the amount and quality of useful information which is produced.

CHAPTER 7

CLOSURE

In this chapter a summary is given of the main results obtained in the present study together with some suggestions for future research.

7.1 Main findings of the present study

In general the aims of devising and testing a numerical calculation procedure for simulating turbulent plume dispersal have been successfully accomplished. The main components of the research may be summarised as follows:

(i) A second-order-closure turbulence model has been developed which can simulate the turbulent dispersal of a two or three dimensional concentration field in a two-dimensional flow field; under stable, neutral or unstable stratification. This task entailed modification and extension to an existing model to account for the effects of thermal stratification on the dissipation rate ϵ of turbulence energy and the turbulent concentration flux $\overline{u_1 c}$. The transport equation for the latter was also extended to allow for the existence of larger differences between the macroscopic length scales of the turbulent eddies and the plume. The modifications introduced resulted in substantial improvements to the predictions of the hydrodynamic and concentration fields.

(ii) A solution procedure has been devised where-by the concentration and hydrodynamic differential conservation

equations are solved on separate grids which are allowed to vary independently in size with downstream distance so as to just encompass the regions of interest. The use of this two-grid system proved to be much more economical than if a single grid has been used, particularly when applied to plume dispersal in the atmospheric boundary layer.

(iii) The predictions of the solution procedure compared favourably with experimental data from both wind-tunnels and atmospheric measurements in a variety of situations. The only situations where relatively large disparities were observed was in the calculation of the lateral dispersal coefficient σ_2 for atmospheric releases. In such cases the predicted values for σ_2 were smaller than those suggested by the semi-empirical correlation of Pasquill; this was attributed to the effect of variation of mean wind direction inherent in Pasquill's results but was not represented in the predictions of the present model.

(iv) An experimental programme provided data on the hydrodynamic (mean and turbulent quantities) and concentration fields for point releases over uniformly-smooth and partially-rough surfaces. These data provided a useful testing ground for the prediction method as well as being of interest in its own right, the latter comment being particularly applicable to the measurements for partially-rough surfaces, which are believed to be novel.

7.2 Suggestions for further work

Proposals for further research in both theoretical and experimental aspects of the dispersal problem are made in

the following sub-sections.

7.2.1 Theoretical proposals

- (i) The present procedure may be extended so as to handle situations where lateral velocities $\bar{U}_2$ exist but are invariant with x_2 . This can be achieved by solving the lateral momentum equation for $\bar{U}_2$ and a further algebraic equation for the Reynolds stress component $\overline{u_2 u_3}$. In this case the Coriolis component of acceleration need not be omitted from the equations in which it appears. Such an extension is straightforward to accomplish, requires no additional three-dimensional storage and will yield interesting predictions of the Eckman spiral.
- (ii) The effects of lateral motion may then be incorporated into the diffusion calculations. In this case, due to the increase of $\bar{U}_2$ with height, lower concentration gradients with x_2 , are bound to exist at larger height. Thus for an economical grid distribution, a sparser grid node distribution (in the lateral direction) should be employed in the top region of the plume than in the lower part. To include such a modification the grid width should be allowed to vary with height; this would lead to a non-orthogonal grid in the $x_2 x_3$ plane, which would necessitate some modification to the concentration transport equation.
- (iii) Insertion and solution of the equations for the variables $\bar{c}^2$ and $\bar{\theta}^2$, which would allow transport effects of these variables to be accounted for in the equations for $\overline{u_1 c}$ and $\overline{u_1 \theta}$ respectively. Accounting for such transport effects could

lead to much better predictions in the immediate vicinity of the source* (for $\overline{u_i c}$) and in regions where large gradients in boundary condition affecting $\overline{\theta^2}$ and $\overline{c^2}$ occur.

(iv) Incorporation of modelled equations for the dissipation rates ϵ_c and ϵ_θ of $\overline{c^2}$ and $\overline{\theta^2}$ respectively would complement the previous suggestion and provide together with $\overline{c^2}$ and $\overline{\theta^2}$ time scales for the temperature and concentration fields respectively. It should be remarked, however, that current belief is that the performance of the equation for the dissipation rate ϵ is itself inadequate and even greater uncertainties enter into the formulation of those for ϵ_c and ϵ_θ .

7.2.2 Experimental proposals

The following studies would be of aid in guiding further theoretical developments:

(i) Measurements of $\overline{c^2}$ and $\overline{u_i c}$:- Such measurements have already been made for the dispersal of heat (i.e. $\overline{\theta^2}$ and $\overline{u_i \theta}$ were determined) but only in situations where the temperature field is two-dimensional (i.e. 'release' from a line source). Performance of similar experiments for point sources might not be feasible because the relatively high source strength required to produce appreciable temperature gradients might provoke unwanted buoyancy effects. Recent developments in measuring concentrations of aerosol particles, released from

*Note that in the present study no comparisons between predictions and experiments were made in the immediate vicinity of the source due to lack of experimental data; hence assessment of the performance of the present model under such circumstances could not be made.

a point source, by laser counting; devices Schon (1978) may allow $\overline{c}^2$ to be obtained directly. In addition insertion of a hot wire probe in the vicinity of the point of particle counting might allow the correlation $\overline{u_1 c}$ to be obtained.

(ii) Measurement of the correlation $\overline{c\theta}$: This might be accomplished by employing the above method, but using the hot-wire probe to measure instantaneous temperature.

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Nomenclature

a', a_3	Turbulence model constants appearing in the modelled equation of the turbulent pollution concentration flux.
a_{ik}	Departure from isotropy tensor, also second order tensor defined by equation (3.84).
a_{jk}^i	Third order tensor defined in equation (3.47).
a_{jl}^{in}	Fourth order tensor defined in equation (3.34).
C	Instantaneous pollutant concentration.
C_m	Maximum pollutant concentration.
c	Fluctuating pollutant concentration.
c_p, c_v	Heat capacity of the fluid at constant volume and constant pressure respectively.
$c_1, c_2, c_3, c_1^i, c_2^i, c_3^i, c_s$	Constants appearing in the modelled Reynolds stress equation.
$c_{1c}, c_{2c}, c_{3c}, c_{1c}^i, c_{2c}^i, c_{3c}^i$	Constants appearing in the modelled turbulent scalar flux equation.
$c_{\epsilon 1}, c_{\epsilon 2}, c_{\epsilon 3}, c_{\epsilon}$	Constants appearing in the modelled dissipation rate equation.
E	Coefficient in the logarithmic law of the wall

for velocity.

E_ϕ	Coefficient in the logarithmic law of the wall for temperature.
E_1, E_2	Output signals (voltages) from hot-wire anemometers.
E_E	Eulerian energy density spectrum.
E_L	Lagrangian energy density spectrum.
Ec_t	Turbulent Eckert number ($u'^2/R\theta'$)
e_{sj}	Cosine of the angle between the axis $o'x'_s$ and ox_j .
Fr_L	Turbulent Froud number based on a length scale L' ($\equiv u'^2/gL'$)
f	Coriolis parameter.
G	Production of turbulence energy by buoyancy action.
G_{ij}	Production of Reynolds stress by buoyancy action.
$G_{k\phi}$	Production of turbulent heat flux by buoyancy effects.
g	Acceleration due to gravity.
H	Heat flux from/to the ground.
K_i	Turbulent concentration diffusivity in i direction.
k	Turbulence kinetic energy.
k_ϕ	Thermal conductivity.
k_s	Equivalent sand roughness.

L	Monin-Obukhov length scale.
$L_i (i=1,2,3), L$	Macroscopic length scales.
ℓ	Turbulence length scale.
ℓ_m	Mixing length.
n_i	Unit vector normal to the ground.
P	Instantaneous pressure, also production of turbulence energy due to mean strain rate.
P_T	Total production rate of turbulence energy.
P_{ij}	Production rate of Reynolds stress due to mean strain rate.
$P_{k\phi}$	Production of turbulent heat flux due to mean strain rate.
$Pe_m (m=n,s,e)$	Cell Peclet number.
Pe_δ	Peclet number based on $\delta (\equiv \delta U_G / \nu_\theta)$.
Pe_λ	Turbulent Peclet number based on $\lambda (\equiv u' \ell / \nu_\theta)$.
Pr_t	Turbulent Prandtl number.
p	Fluctuating pressure.
Q	Pollutant source strength.
Q'	Pollutant source strength/unit length.
q	Data acquisition rate.

R	Gas constant, also correlation coefficient ($\equiv \overline{u_1 u_3} / \overline{u_3^2} \overline{u_1^2}$)
R_C	Ratio between time scale of fluctuating concentration and velocity fields, also total residual.
R	Ratio between time scale of fluctuating temperature and velocity fields.
R_E	Eulerian auto-correlation coefficient.
R_L	Lagrangian auto-correlation coefficient.
Re_δ	Reynolds number ($\equiv U_G \delta / \nu$).
Re_ℓ	Turbulence Reynolds number based on ℓ ($\equiv u' \ell / \nu$).
Re_λ	Turbulence Reynolds number based on λ ($\equiv u' \lambda / \nu$).
Rf	Flux Richardson number.
Rf_δ	Over-all Richardson number.
RO_δ	Rossby number ($\equiv f \delta / U_G$).
RO_ℓ	Turbulence Rossby number based on ℓ ($\equiv u' f / \ell$).
r_i	Position vector in x_1, x_2, x_3 coordinate system.
S_c	Source term of pollutant concentration.
S_{ij}	Lagrangian correlation ($\overline{V_i(t) V_j(t+\xi)}$).
S_ϕ	Auto-correlation of ϕ .
Sc_t	Turbulent Schmidt number.

s_{ij}	Fluctuating rate of strain.
T	Averaging time.
T_m	Time scale of mean quantities.
U_i	Instantaneous velocity in the i direction.
$U_{1\infty}$	Main-stream velocity.
U_G	Geostrophic wind velocity
u_i	Fluctuating velocity in the i direction.
u'	Root mean square of $2k$.
u'_j	Root mean square of u_j .
u_*	Friction velocity.
v_i	Fluctuating Lagrangian velocity in the i direction.
W	Mean velocity scale.
w	Turbulent velocity scale
x_3^h	Vertical distance from the ground to upper boundary of the plume.
x_3^l	Vertical distance from the ground to lower boundary of the plume.
x_3	Vertical dimension of the plume.
x_2	Lateral width of the plume.

x_1, x_2, x_3	Stream-wise, vertical and lateral directions in the Cartesian rotating frame of reference.
$o'x_1', x_2', x_3'$	'Inertial' (not rotating with the earth about its axis however follows the earth's orbit about the sun) with $o'x_3'$ (axis of rotation) pointing north and the origin o' at the centre of the earth.
x_o	Roughness parameter.
y_1, y_2, y_3	Lagrangian Cartesian coordinates.
z_n	Position vector of the flow domain in $o'x_1', x_2', x_3'$.

Greek symbols

α_{ik}	Coriolis parameter ($\equiv -2\Omega\epsilon_{ijk} e_{sj} \lambda_s$).
β'	Constant appearing in the logarithmic-linear law of the wall.
β_i	Gravitational parameter (gn_i/θ_m).
Γ_t	Turbulent thermal diffusivity in the vertical direction.
Γ_i^ϕ	Turbulent diffusivity of ϕ in i direction.
γ_c	Molecular, pollutant species diffusivity.
γ_ϕ	Molecular thermal diffusivity.
δ	Boundary layer thickness.
δ_c	Plume thickness.

δ_i	Boundary layer thickness at point of injection.
δ_{ij}	Kronecker delta.
ϵ	Dissipation rate of turbulence kinetic energy.
ϵ_c	Dissipation rate of the mean square of the fluctuating concentration.
ϵ_ϕ	Dissipation rate of the mean square of the fluctuating temperature.
ϵ_{ijk}	Permutation tensor.
η	Kolmogorov length scale.
η_1, η_2, η_3	Coordinate system used to describe the concentration grid.
θ	Instantaneous temperature.
θ_m	Reference temperature.
θ	Fluctuating temperature.
θ'	Root mean square to fluctuating temperature.
θ_*	Scaling temperature
κ	Von-Karman constant to the logarithmic law.
κ_1, κ_2	Coefficients used in signal processing of hot-wire outputs.
Λ_E	Integral Eulerian time scale.
Λ_L	Integral Lagrangian time scale.

λ	Taylor microscale.
λ_2	Lateral distance from plane of symmetry to the location where the mean concentration is half the maximum.
λ_3	Vertical distance from the ground to the location where the mean concentration is half the maximum.
μ	Laminar viscosity.
μ_t	Turbulent viscosity.
ν	Kinematic viscosity.
ξ_1, ξ_2, ξ_3	Coordinate system used to define hydrodynamic grid.
ρ	Density.
σ_i	Standard deviation of y_i .
τ	Shear stress.
ϕ_{ij}	Pressure-velocity gradient correlation.
$\phi_{ijm} (m=1,2,3,4)$	Components of ϕ_{ij} (excluding wall effects).
$\phi_{ijmw} (m=1,2,3)$	Component of ϕ_{ij} due to wall effects.
ϕ_{ic}	Pressure-scalar gradient correlation.
$\phi_{icm} (m=1,2,3,4)$	Components of ϕ_{ic} (excluding wall effects).

$\phi_{icmw}^{(m=1,2,3)}$ Components of ϕ_{ic} due to wall effects.

Ω Frequency of earth's rotation about its axis.

Overbars indicate averaged quantities.

APPENDIX A1

COMMENT ON PARAMETERS CHOSEN BY SUTTON TO DESCRIBE
THE CORRELATION COEFFICIENT R_L

It is well known that the value of the correlation coefficient R_L is affected directly by the length scale* of the turbulent regime considered (c.f. Townsend (1976)); the length scale in turn is affected by factors such as physical dimensions of the flow domain (e.g. distance from the ground for a boundary layer flow), degree and type of thermal stratification etc. Hence to estimate R_L enough information to imply a length scale must be available.

Now, the parameters chosen by Sutton to describe R_L comprise $\bar{u}_{(i)}^2$, ξ and $u_* x_o$ (or v); none of these variables, or a combination of them, is capable of providing the required turbulence length scale, and therefore further parameters are needed. One such parameter for example is the dissipation rate ϵ (for neutral, near wall flows this is approximately equal to $u_*^3/\kappa y$) which with $\bar{u}_{(i)}^2$ can yield a turbulent length scale.

*Note that time and length scales are closely related.

APPENDIX B1

MODIFICATION OF A CONCENTRATION FIELD TO ACCOUNT FOR LONG AVERAGING TIMES

The following is an ad-hoc model that generates long time (T_L say) average concentration field from results averaged over a shorter time interval T (see also Naden and Leeds (1972)).

It is assumed that the plume which is a result of averaging over time T is being moved intact, continuously in the lateral direction by the action of large scale motions. The axis of the plume (which is considered to coincide with the mean wind direction (β) averaged over T) is envisaged to be randomly fluctuating with an angle θ about the axis aligned to the mean wind direction (β_L) which is averaged over time T_L where the axis passes through the source as shown in Figure B1.1. If we now consider a series of averaging time intervals, each of duration T , we will obtain corresponding values of θ which have a normalised frequency distribution function $f(\theta)$.

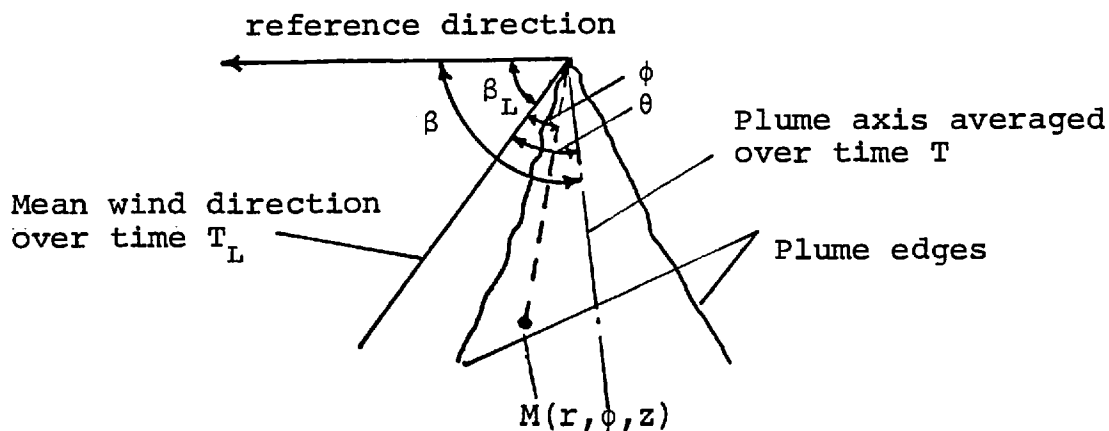


Figure B1.1

The value of the concentration $\bar{\bar{C}}(r, \phi, z)$, averaged over a time T_L , at a point $M(r, \phi, z)$ (in cylindrical co-ordinates with z axis parallel to x_3), say, is then taken as the weighted average of the short time averaged plume concentration over its different orientations. The weight being decided by the relative frequency of its angle θ . Mathematically this is written as

$$\bar{\bar{C}}(r, \phi, z) = \int_0^{2\pi} f(\theta) \bar{C}(r, \theta - \phi, z) d\theta$$

where $\bar{C}$ are the values of concentration averaged over time T .

The shape of the function $f(\theta)$ could be obtained from atmospheric observations.

APPENDIX C1

ESTIMATION OF THE ORDER OF MAGNITUDE OF TERMS APPEARING
IN THE DISSIPATION RATE EQUATION

In evaluating the order of magnitude of the terms in the dissipation equation, the following relation deduced from Tennekes and Lumley (1974) (see also Siess (1975)) are useful*

$$|\phi_{,i}| \sim \phi/\lambda \quad (C1.1)$$

$$|\phi_{,ij}| \sim \phi/\lambda\eta \quad (C1.2)$$

where ϕ is any of the fluctuating variables[‡] $u_i, \theta, \dots$ etc.

As mentioned by Lumley (1975), roughly speaking instantaneous quantities appearing in the correlations lie either in the energy-containing range or the dissipation range with the former having a characteristic frequency u'/l and the latter u'/λ . The correlation coefficient between two quantities from the same frequency range is of order

*| | denotes the root mean square value of the variable.

[‡]Strictly speaking different length scales λ_θ and η_θ must be used when (C1.1) and (C1.2) are employed to find $|\theta_{,i}|$ and $|\theta_{,ij}|$ (c.f. Tennekes and Lumley (1971)).

unity while the correlations between different frequencies is of the order of the time scale ratio λ/l .

At high turbulence Reynolds number the two above-mentioned frequency ranges are decoupled (only linked through spectral energy transfer) and all anisotropy is confined to the low-frequency end of the energy spectrum. Therefore all correlations having their main energy contribution at high wave numbers are expected to be close to isotropic. The degree of anisotropy, at a certain wave number, was argued by Tennekes and Lumley (1974) to be proportional to the ratio between the strain rate of the larger eddies and the strain rate of the eddies whose anisotropy is being examined. Hence the non isotropy of the eddies at the dissipation range would be proportional to λ/l .

Now it can be shown by revolving the coordinate system that correlations of the following form are zero in isotropic turbulence

$$\overline{u_{i,1}\phi_{,1}} = 0 \quad (C1.3)$$

$$\overline{u_{i,1}u_{j,m}} = 0 \quad \begin{array}{l} \text{when } l = m \text{ and } i \neq l \\ \text{or } i = j \text{ and } l \neq m \end{array} \quad (C1.4)$$

where ϕ is either of the scalars p or θ . Since correlations in (C1.3) and (C1.4) are expected to have their main contribution of energy in the dissipation range of the energy spectrum, their values, in non-isotropic flows, will be different from zero only in response to the degree of anisotropy in the dissipation range: thus their order of

magnitude* is:

$$\overline{u_{i,1} \phi_{,1}} \sim \frac{u \phi}{\lambda^2} \frac{\lambda}{l}$$

$$\overline{u_{i,1} u_{j,m}} \sim \frac{u^2}{\lambda^2} \frac{\lambda}{l} \quad \begin{array}{l} \text{when } l = m \text{ and } i \neq j \\ \text{or } i = j \text{ and } l \neq m \end{array}$$

From the above arguments the order of magnitude of each of the terms in equation (3.8) can then be estimated as:

$$(i) \quad \partial \epsilon / \partial t \sim \nu u'^3 / l T$$

$$(ii) \quad \overline{U_j \epsilon_{,j}} \sim u'^4 / l^2$$

$$(iii)^{\ddagger} \quad \nu (\overline{u_{i,1} u_{j,1}} + \overline{u_{1,i} u_{1,j}}) \overline{U_{i,j}} \sim \nu u'^3 / \lambda l^2$$

$$(iv) \quad \nu (\overline{u_{i,j} u_{i,1} u_{j,1}}) \sim \nu u'^3 / \lambda^3$$

$$(v) \quad \overline{(\nu u_{i,j1})^2} \sim \nu^2 u'^2 / \lambda^2 \eta^2$$

$$(vi)^+ \quad \nu (\overline{u_j (u_{i,1})^2})_{,j} \sim \nu u'^3 / \lambda^2$$

*For a more rigorous analysis for estimating the order of magnitude of $\overline{u_{i,1} u_{j,m}}$ see Lumley (1970).

$\ddagger$ The relation $U_{i,j} \delta_{ij} = 0$ (for an incompressible flow) was employed.

$^+$ This term can be written as $\overline{u_j \nu (u_{i,1})^2_{,j}}$ and thus can be assumed to be well correlated since u_j and the diffusion term $(u_{i,1})^2_{,j}$ are approximately from the same frequency range (see Tennekes and Lumley (1974)).

$$\begin{array}{ll}
 \text{(vii)*} & \frac{\nu}{\rho} \overline{u_{i,1}^p},_1 \sim \nu u'^3/\lambda l^2 \\
 \text{(viii)} & \nu \overline{u_{j,i,1} u_{i,1j}} \sim \nu u'^3/l^3 \\
 \text{(ix)} & \nu \varepsilon_{,jj} \sim \nu^2 u'^2/\lambda^2 l^2 \\
 \text{(x)} & \nu \beta_i \overline{\theta_{,1} u_{i,1}} \sim \nu \beta \frac{\theta u'}{\lambda l} \\
 \text{(xi)} & \nu \alpha_{ik} \overline{u_{k,1} u_{i,1}} \sim \nu \alpha \frac{u'^2}{\lambda l}
 \end{array}$$

where $\beta = |\beta_i|$ and $\alpha = |\alpha_{ik}|$.

Comparing all the terms to $\nu u'^3/\lambda^3$ and employing relations (3.12) to (3.14) we obtain

$$\begin{array}{ll}
 \text{Term (i)} & \sim Re_1^{-1/2} l/u'T \\
 \text{Term (ii)} & \sim Re_1^{-1/2} \\
 \text{Term (iii)} & \sim Re_1^{-1} \\
 \text{Term (iv)} & \sim 1 \\
 \text{Term (v)} & \sim 1 \\
 \text{Term (vi)} & \sim Re_1^{-1/2} \\
 \text{Term (vii)} & \sim Re_1^{-1} \\
 \text{Term (viii)} & \sim Re_1^{-1.5} \\
 \text{Term (ix)} & \sim Re_1^{-1.5} \\
 \text{Term (x)} & \sim Rf Re_1^{-1} \\
 \text{Term (xi)} & \sim Ro_1^{-1} Re_1^{-1/2}
 \end{array}$$

*The order of magnitude of the pressure fluctuation is assumed to be $\rho u'^2$ (in isotropic turbulence at high Reynolds numbers $p = \rho u'^2$, c.f. Hinze (1975)).

APPENDIX C2

CALCULATION OF a_{jj}^{in} , a_{jj}^i and a_{ii}

C2.1 Calculation of a_{jj}^{in}

a_{jj}^{in} is defined as

$$a_{jj}^{in} = -\frac{1}{2\pi} \int \frac{\partial^2 \overline{u_i u_n'}}{\partial \zeta_1 \partial \zeta_j} \frac{dV'}{|\underline{r}|} \quad (C2.1)$$

where

$$|\underline{r}| = r = \sqrt{\zeta_i \zeta_i} \quad (C2.2)$$

$$dV' = d\zeta_1 d\zeta_2 d\zeta_3 \quad (C2.3)$$

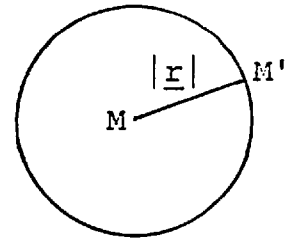


Figure C2.1

In equation (C1.1) u_i is calculated at $\underline{r} = 0$ (point M) while u_n' is considered at a point M' having a relative (to M) position vector $\underline{r}$ (see figure C1).

If the variable considered is independent of direction i.e. in isotropic turbulence then from (C2.2)

$$\frac{\partial}{\partial \zeta_i \partial \zeta_j} = \frac{\delta_{ij}}{r} \frac{\partial}{\partial r} - \frac{\zeta_i \zeta_j}{r^3} \frac{\partial}{\partial r} + \frac{\zeta_i \zeta_j}{r^2} \frac{\partial^2}{\partial r^2}$$

thus

$$\frac{\partial}{\partial \zeta_i \partial \zeta_i} = \frac{2}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \quad (C2.4)$$

Transforming the integral in A1.1 to spherical coordinates and inserting (C2.4) into (C2.1), there results

$$a_{jj}^{in} = -\frac{1}{2\pi} \int_0^\infty \int_0^{2\pi} \int_0^\pi \left(\frac{2}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \right) \overline{u_i u_n'} r \sin\theta d\theta d\phi dr$$

integrating over θ and ϕ we obtain

$$a_{jj}^{in} = -2 \int_0^\infty \left(\frac{2}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \right) \overline{u_i u_n'} r dr$$

integrating by parts:

$$a_{jj}^{in} = -2 \left(2 \overline{u_i u_n'} \Big|_0^\infty + r \frac{\partial}{\partial r} \overline{u_i u_n'} \Big|_0^\infty - \overline{u_i u_n'} \Big|_0^\infty \right)$$

Now at $r = \infty$, $\overline{u_i u_n'}$ is equal to zero and at $r = 0$, $\overline{u_i u_n'} = \overline{u_i u_n}$.

Therefore

$$a_{jj}^{in} = 2 \overline{u_i u_n} \quad (C2.5)$$

C2.2 Calculation of a_{jj}^i

a_{jj}^i is defined as

$$a_{jj}^i = -\frac{1}{4\pi} \int \frac{\partial^2 \overline{u_i}}{\partial \xi_i \partial \xi_j} \frac{dv'}{|\underline{r}|} \quad (C2.6)$$

with (C2.4) and by transforming to spherical coordinates

$$a_{jj}^i = -\frac{1}{4\pi} \int_0^\infty \int_0^{2\pi} \int_0^\pi \frac{2}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \overline{\theta u_i'} r \sin\theta d\theta d\phi dr$$

by carrying out the integration and noting that $\overline{\theta u_i'}$ is equal to zero with $r = \infty$ and $\overline{\theta u_i'} = \overline{\theta u_i'}$ at $r = 0$ we obtain

$$a_{jj}^i = \overline{\theta u_i'} \quad (C2.7)$$

C2.3 Calculation of a_{ii}

a_{ik} for homogeneous turbulence can be written as

$$a_{ik} = -\frac{1}{4\pi} \int_{vol} \frac{\partial \overline{\theta' \theta}}{\partial \zeta_i \partial \zeta_k} \frac{dV'}{|\underline{r}|}$$

With a similar procedure to the above and by noting that $\overline{\theta \theta'}$ is equal to zero at $r = \infty$ and $\overline{\theta \theta'} = \overline{\theta^2}$ at $r = 0$ we get

$$a_{ii} = \overline{\theta^2} \quad (C2.8)$$

APPENDIX C3

DERIVATION OF EXPRESSIONS FOR ϕ_{ij2} , ϕ_{ij3} AND ϕ_{ic2} USING TENSOR INVARIANT THEORY

The condition that a certain quantity is invariant under coordinate system transformation aids in giving general functional dependence a more specific form; this is basically what invariant theory is concerned with. This theory will be employed here to aid in calculating a_{lj}^{im} and a_{ij}^i and hence to calculate ϕ_{ij2} , ϕ_{ij3} and ϕ_{ic2} .

C3.1 Calculation of ϕ_{ij2}

a_{lj}^{im} is defined as

$$a_{lj}^{mi} = F_{imlj}(\overline{u_k u_s}) \quad (C3.1)$$

If (C3.1) is multiplied by the arbitrary vectors A_l , B_j , C_i and D_m and by contracting* over i , n , l and j the left hand side is reduced to an invariant that is multilinear in A_l , B_j , C_i and D_m . Consequently the right hand side should also be an invariant, multilinear in the arbitrary vectors mentioned.

This is expressed mathematically as

$$a_{lj}^{mi} A_l B_j C_i D_m = F(\overline{u_R u_s} \overline{u_s u_k}, \overline{u_k u_s} \overline{u_s u_j}, \overline{u_j u_n} \overline{u_n u_m}, \dots)$$

*It is noted that c contraction is permissibly since we are employing a cartesian coordinate system.

$$\overline{u_k u_s^n} A_k B_s D_i C_i \dots) \quad (C3.2)$$

where $\overline{u_k u_s^n}$ is the n^{th} power of the tensor $\overline{u_k u_s}$ and is defined as

$$\overline{u_k u_s^n} = \overline{u_k u_m} \overline{u_m u_1} \dots \overline{u_1 u_s}$$

with n factors. According to the Cayley-Hemiton theory (c.f. Lumley (1970)), in three dimensional space, only up to the value of $n = 2$ are independent; hence we can write

$$\begin{aligned} a_{lj}^{mi} \overline{u_k u_s} A_l B_j C_i D_m &= a \overline{u_k u_s^0} A_s B_k D_m C_m + b \overline{u_k u_s} A_s B_k D_m C_m + \\ &+ c \overline{u_k u_s^2} A_s B_k D_m C_m + d \overline{u_k u_s^0} A_s D_k B_j C_j + e \overline{u_k u_s} A_s D_k B_j C_j + \\ &+ f \overline{u_k u_s^2} A_s D_k B_j C_j + g \overline{u_k u_s^0} A_s C_k B_j D_j + h \overline{u_k u_s} A_s C_k B_j D_j + \\ &+ i \overline{u_k u_s^2} A_s C_k B_j D_j + j \overline{u_k u_s^0} B_s C_k A_m D_m + k \overline{u_k u_s} B_s C_k A_m D_m + \\ &+ l \overline{u_k u_s^2} B_s C_k A_m D_m + m \overline{u_k u_s^0} B_s D_k A_l C_l + n \overline{u_k u_s} B_s D_k A_l C_l + \\ &+ o \overline{u_k u_s^2} B_s D_k A_l C_l + p \overline{u_k u_s} C_s D_k A_l B_l + q \overline{u_k u_s} C_s D_k A_l B_l + \\ &+ r \overline{u_k u_s^2} C_s D_k A_l B_l \end{aligned} \quad (C3.3)$$

where the coefficients $a, b, c \dots$ etc. are functions of the invariants of $\overline{u_k u_s}$ and $\overline{u_k u_s^0}$ is defined as

$$\overline{u_k u_s^0} = \delta_{ks}$$

By cancelling the arbitrary vectors from both sides of (C3.3) we get

$$\begin{aligned} a_{lj}^{mi} = & a\delta_{lj}\delta_{im} + b\overline{u_j u_l}\delta_{im} + c\overline{u_n u_j}\overline{u_n u_l}\delta_{im} + d\delta_{ml}\delta_{ij} + \\ & e\overline{u_m u_l}\delta_{ij} + f\overline{u_m u_n}\overline{u_n u_l}\delta_{ij} + g\delta_{il}\delta_{jm} + h\overline{u_i u_l}\delta_{jm} + \\ & i\overline{u_i u_n}\overline{u_n u_l}\delta_{jm} + j\delta_{ij}\delta_{ml} + s\overline{u_i u_j}\delta_{ml} + l\overline{u_i u_n}\overline{u_n u_j}\delta_{ml} + \\ & m\delta_{mj}\delta_{li} + n\overline{u_m u_j}\delta_{li} + o\overline{u_m u_n}\overline{u_n u_j}\delta_{li} + p\delta_{mi}\delta_{lj} + q\overline{u_m u_i}\delta_{lj} \\ & + r\overline{u_m u_n}\overline{u_n u_i}\delta_{lj} \end{aligned} \quad (C3.4)$$

From the kinematic constraints $a_{lj}^{mi} = a_{lj}^{im} = a_{jl}^{im}$ we get

$$d + j = g + m \quad (C3.5)$$

$$h = s = n = e \quad (C3.6)$$

$$l = o = i = f \quad (C3.7)$$

Putting $d + j \equiv u$ and $a + p = v$ we get

$$\begin{aligned} a_{lj}^{mi} = & v\delta_{lj}\delta_{im} + b\overline{u_j u_l}\delta_{im} + c\overline{u_n u_j}\overline{u_n u_l}\delta_{im} + u(\delta_{ml}\delta_{ij} + \\ & \delta_{il}\delta_{jm}) + h(\overline{u_m u_l}\delta_{ij} + \overline{u_i u_l}\delta_{jm} + \overline{u_i u_j}\delta_{ml} + \overline{u_m u_j}\delta_{li}) + \end{aligned}$$

$$\begin{aligned}
 & f(\overline{u_m u_n u_n u_l} \delta_{ij} + \overline{u_i u_n u_n u_j} \delta_{ml} + \overline{u_i u_n u_n u_l} \delta_{jm} + \overline{u_m u_n u_n u_j} \delta_{li}) \\
 & + q \overline{u_m u_i} \delta_{lj} + r \overline{u_m u_n u_n u_i} \delta_{lj}
 \end{aligned} \tag{C3.8}$$

By retaining only the linear terms and applying the constant $a_{li}^{mi} = 0$ we obtain

$$0 = \delta_{lm} (v + 4u + h \overline{u_i^2}) + u_m u_l (b + 5h + q)$$

or

$$v + 4u + h \overline{u_i^2} = 0 \tag{C3.9}$$

and

$$b + 5h + q = 0 \tag{C3.10}$$

From $a_{jj}^{mi} = 2 \overline{u_m u_i}$ and (C3.8) we have

$$2 \overline{u_m u_i} = \delta_{im} (3v + b \overline{u_i^2} + 2u) + \overline{u_m u_i} (4h + 3q)$$

from which

$$3v + b \overline{u_i^2} + 2u = 0 \tag{C3.11}$$

and

$$4h + 3q = 2 \tag{C3.12}$$

(C3.9) - (C3.12) give five unknowns in four equations;
hence by solving these equations in terms of b there results

$$u = \frac{(20b + 6)}{55} \frac{\bar{u}_i^2}{2}$$

$$v = -\frac{(50b + 4)}{55} \frac{\bar{u}_i^2}{2}$$

$$q = \frac{(4b + 10)}{11}$$

$$h = -\frac{(3b + 2)}{11}$$

Thus from (C3.8) we get

$$\begin{aligned} a_{lj}^{mi} = & c_2 \bar{u}_j \bar{u}_l \delta_{im} + \frac{(20c_2 + 6)k}{55} (\delta_{ml} \delta_{ij} + \delta_{il} \delta_{jm}) - \\ & \frac{(3c'_2 + 2)}{11} (\bar{u}_m \bar{u}_l \delta_{ij} + \bar{u}_i \bar{u}_l \delta_{jm} + \bar{u}_i \bar{u}_j \delta_{ml} + \bar{u}_m \bar{u}_j \delta_{li}) + \\ & \frac{(4c'_2 + 10)}{11} \bar{u}_m \bar{u}_i \delta_{lj} - \frac{(50c_2 + 4)k}{55} \delta_{lj} \delta_{im} \end{aligned} \quad (C3.13)$$

where b was replaced by c'_2 .

Now

$$\phi_{ij2} = \bar{u}_{1,m} a_{lj}^{mi} \quad (c3.14)$$

Using equation (C3.13) and applying the continuity equation $\bar{U}_{i,i} = 0$, we arrive at the following equation for ϕ_{ij}

$$\begin{aligned} \phi_{ij2} = & c_2' \overline{u_j u_1} \bar{U}_{1,i} - \frac{(30c_2' - 2)k(\bar{U}_{i,j})}{55} - \frac{(3c_2' + 2)}{11} \\ & (\overline{u_m u_1} \bar{U}_{1,m} \delta_{1j} + \overline{u_i u_1} \bar{U}_{1,j} + \overline{u_m u_j} \bar{U}_{i,m}) + \frac{(4c_2' + 10)}{11} \overline{u_m u_i} \bar{U}_{j,m} \end{aligned} \quad (C3.15)$$

Adding ϕ_{ji2} to ϕ_{ij2} and collecting terms we finally obtain

$$\begin{aligned} (\phi_{ij} + \phi_{ji})_2 = & -\frac{(c_2' + 8)}{11} \{P_{ij} - \frac{2P\delta_{ij}}{3}\} - \frac{(30c_2' - 2)}{55} \\ & k\{\bar{U}_{i,j} + U_{j,i}\} - \frac{(8c_2' - 2)}{11} (D_{ij} - \frac{2P\delta_{ij}}{3}) \end{aligned} \quad (C3.16)$$

C3.2 Calculation of ϕ_{ij3}

ϕ_{ij3} is defined as

$$\phi_{ij3} = \beta_n a_{nj}^i \quad (C3.17)$$

where a_{nj}^i is the third order tensor:

$$a_{nj}^i = G_{inj} (\overline{u_k \theta}) \quad (C3.18)$$

By following a similar procedure to that used in the derivation of a_{lj}^m , it can be shown that a_{nj}^i can be written as:

$$a_{nj}^i = d\overline{u_i\theta}\overline{u_j\theta}\overline{u_R\theta} + a\overline{u_n\theta}\delta_{ji} + b\overline{u_j\theta}\delta_{in} + c\overline{u_i\theta}\delta_{jn} \quad (C3.19)$$

where d , a , b and c are functions of the invariants of $\overline{u_i\theta}$.

From constraint (3.48) and equation (C3.19) we get

$$a = b = e \text{ (say)}$$

Employing the continuity constraint (3.49) and by retaining only linear terms (of $\overline{u_i\theta}$) in equation (C3.19), the latter yields

$$\overline{u_i\theta}(4e + c) = 0$$

or

$$c = -4e \quad (C3.20)$$

With relation (3.50), (C3.20) and (C3.19) there results

$$\overline{u_i\theta} = 2a\overline{u_i\theta} + 3c\overline{u_i\theta}$$

or

$$2e + 3c = 1 \quad (C3.21)$$

hence with (C3.20)

$$e = -0.1 \quad (C3.22)$$

and

$$c = 0.4 \quad (C3.23)$$

With these results a_{nj}^i can be written as

$$a_{nj}^i = 0.4 \overline{u_i \theta} \delta_{nj} - 0.1 (\overline{u_n \theta} \delta_{ji} + \overline{u_j \theta} \delta_{in}) \quad (C3.24)$$

and ϕ_{ij3} becomes

$$\phi_{ij3} = 0.4 \beta_j \overline{u_i \theta} - 0.1 (\beta_n \overline{u_n \theta} \delta_{1j} + \beta_i \overline{u_j \theta}) \quad (C3.25)$$

From which

$$(\phi_{ij} + \phi_{ji})_3 = 0.3 (G_{ij} - \frac{2}{3} \delta_{ij} G) \quad (C3.26)$$

C3.3 Calculation of ϕ_{ic2}

The vector ϕ_{ic2} is defined by

$$\phi_{ic2} = 2a_{1i}^n \overline{U}_{1,n} \quad (C3.27)$$

where a_{1i}^n is given by equation (C3.24), hence

$$\phi_{ic2} = \overline{U}_{1,n} \{0.8 \overline{u_n \theta} \delta_{1i} - 0.2 (\overline{u_1 \theta} \delta_{ni} + \overline{u_i \theta} \delta_{1n})\} \quad (C3.28)$$

by employing the continuity equation $\overline{U}_{1,1} = 0$ we get

$$\phi_{ic2} = 0.8 \overline{U}_{1,n} \overline{u_n \theta} - 0.2 \overline{U}_{1,i} \overline{u_1 \theta} \quad (C3.29)$$

APPENDIX C4

MODELLING OF THE TRANSPORT EQUATION OF THE CORRELATION $\overline{c\theta}$

The equation for the correlation $\overline{c\theta}$ can be derived by multiplying the transport equation of c by θ and adding to the result, the equation of θ multiplied by c . By time averaging and neglecting molecular diffusion the following transport equation for $\overline{c\theta}$ is obtained.

$$\begin{array}{ccccccc} \text{I} & & \text{II} & & \text{III} & & \text{IV} \\ \overline{c\theta}_{,t} + \overline{u_j c\theta}_{,j} = & -(\overline{u_j \theta \overline{c}}_{,j} + \overline{u_j c \overline{\theta}}_{,j}) & - & (\overline{u_j c \theta})_{,j} & - & & \\ & & \text{V} & & & & \\ & & (\gamma_\theta + \gamma_c) \overline{c_{,i} \theta_{,i}} & & & & \end{array} \quad (C4.1)$$

The terms in equation (C4.1) can be identified as follows.

Term I = temporal change term

Term II = convection by mean motion

Term III = production or destruction term by the action of the interaction of turbulent heat and concentration fluxes with the mean concentration and temperature gradient respectively. (note that the two terms in III will almost always have the same sign)

Term IV = diffusion of $\overline{c\theta}$ by turbulent motion

Term v = dissipation term by molecular action

In principle the latter term (i.e. term V), can acquire different signs relative to $\overline{\theta c}$ and thus act as a production or destruction term in equation (C4.1). The arguments in favour of term V being a destruction term, however, are

that: when term III acts as a production term there must be a mechanism to curb $\overline{c\theta}$ from going to infinity, and that can only be term V (the diffusion term merely transports $\overline{c\theta}$ from one region to another). If on the other hand term III becomes a destruction term of $\overline{c\theta}$, then it is improbable that term V can be responsible for providing energy that would maintain $\overline{c\theta}$, this is because $\overline{c_{,i}\theta_{,i}}$ is expected to have its major energy concentrated at a much higher wave number than that of $\overline{\theta c}$ (this can be shown by examining the Fourier transforms of these correlations) and hence any transform of energy from $\overline{c_{,i}\theta_{,i}}$ to $\overline{\theta c}$ would have to be made up the energy spectrum of the latter which is unlikely*.

The only term that needs modelling in equation (C4.1) is term V. A transport equation could be constructed to this correlation (similar to that of ϵ) however for simplicity term IV is modelled as follows:

$$-(v_c + v_\theta) \overline{c_{,j}\theta_{,j}} = -b \overline{\theta c} / t_{c\theta} \quad (C4.2)$$

where b is a constant and $t_{c\theta}$ is a timescale. This form was chosen so that term V is to act as a dissipation term and hence must have a sign which is always, opposite to that of $\overline{\theta c}$; it must also have the same dimension as the original term and furthermore must be a scalar.

The time scale $t_{c\theta}$ more likely would contain some weighing from the thermal and concentration turbulence

*If any resemblance between the spectrum of $\overline{c\theta}$ and that of k is to be assumed.

fields. Here only the former will be used and since that is assumed proportional to the time scale of the turbulent motion hence term V becomes

$$\text{Term V} = -a \frac{\epsilon}{k} \overline{\theta c} \quad (\text{C4.3})$$

where a is another constant. Substituting (C4.3) into (C4.1) and neglecting transport and temporal change terms in the latter, there results

$$\overline{\theta c} = -a' \frac{k}{\epsilon} (\overline{u_j \theta c}_{,j} + \overline{u_j c \theta}_{,j}) \quad (\text{C4.4})$$

where $a' = 1/a$.

APPENDIX D1

DERIVATION OF THE FINITE DIFFERENCE EQUATION OF $\bar{C}$

The partial differential equation of $\bar{C}$ reads:

$$\begin{array}{cccc}
 \text{I} & \text{II} & \text{III} & \text{IV} \\
 \frac{\partial \bar{U}_1 \bar{C}}{\partial x_1} - \frac{\eta_2}{\bar{x}_2} \frac{dx_2}{d\eta_1} \frac{\partial}{\partial \eta_2} \bar{U}_1 \bar{C} - \frac{\eta_3}{\bar{x}_3} \frac{dx_3}{d\eta_1} \frac{\partial \bar{U}_1 \bar{C}}{\partial \eta_3} - \frac{1}{\bar{x}_3} \frac{dx_s^1}{d\eta_1} \frac{\partial}{\partial \eta_3} \bar{U}_1 \bar{C} + \\
 \\
 \text{V} & \text{VI} & \text{VII} & \\
 \frac{1}{\bar{x}_3} \frac{\partial \bar{U}_3 \bar{C}}{\partial \eta_3} = \frac{1}{\bar{x}_2} \frac{\partial}{\partial \eta_2} \frac{\bar{K}_2 \partial \bar{C}}{\bar{x}_2 \partial x_2} + \frac{1}{\bar{x}_3} \frac{\partial}{\partial \eta_3} \frac{\bar{K}_2 \partial \bar{C}}{\bar{x}_3 \partial x_3} + \bar{S}_c & & & (D1.1)
 \end{array}$$

Integrating the terms in equation (D1.1) over the control volume in Figure 4.3 we get*

$$\begin{aligned}
 \int_{\text{vol}} \text{I } J d\eta_1 d\eta_2 d\eta_3 &= \iiint \frac{\partial \bar{U}_1 \bar{C}}{\partial \eta_1} x_2 x_3 d\eta_1 d\eta_2 d\eta_3 \\
 &= \iint \left[\bar{U}_1 \bar{C} x_2 x_3 \Big|_u^d - \int \bar{U}_1 \bar{C} \left(\frac{dx_2}{d\eta_1} x_3 + \frac{dx_3}{d\eta_1} x_2 \right) d\eta_1 \right] d\eta_2 d\eta_3 \\
 \int_{\text{vol}} \text{II } J d\eta_1 d\eta_2 d\eta_3 &= - \iint \left[\bar{U}_1 \bar{C} \eta_2 \Big|_w^e - \int \bar{U}_1 \bar{C} d\eta_2 \right] \frac{dx_2}{d\eta_1} x_3 d\eta_1 d\eta_3 \\
 \int_{\text{vol}} \text{III } J d\eta_1 d\eta_2 d\eta_3 &= - \iint \left[\eta_3 \bar{U}_1 \bar{C} \Big|_s^n - \int \bar{U}_1 \bar{C} d\eta_3 \right] x_2 \frac{dx_3}{d\eta_1} d\eta_1 d\eta_2
 \end{aligned}$$

*J = $\epsilon_{ijk} \frac{\partial x_i}{\partial \eta_1} \frac{\partial x_j}{\partial \eta_2} \frac{\partial x_k}{\partial \eta_3} = x_2 x_3$

$$\int_{vol}^{IV} J d\eta_1 d\eta_2 d\eta_3 = - \int \int \bar{U}_3 \bar{C} \Big|_s^n X_2 \frac{dX_s^1}{d\eta_1} d\eta_1 d\eta_3$$

$$\int_{vol}^V J d\eta_1 d\eta_2 d\eta_3 = \int \int \bar{U}_3 \bar{C} \Big|_s^n X_2 d\eta_1 d\eta_2$$

$$\int_{vol}^{VI} J d\eta_1 d\eta_2 d\eta_3 = \int \int K_2 \frac{\partial C}{\partial \eta_2} \Big|_w^e X_3 \frac{dX_2}{\bar{X}_2} d\eta_1 d\eta_3$$

$$\int_{vol}^{VII} J d\eta_1 d\eta_2 d\eta_3 = \int \int K_3 \frac{\partial C}{\partial \eta_3} \Big|_s^n X_2 \frac{dX_2}{\bar{X}_3} d\eta_1 d\eta_2$$

By employing the mean value theorem and collecting terms there results

$$(\bar{U}_1 \bar{C} X_2 X_3 \Delta \eta_2 \Delta \eta_3)_d - (\bar{U}_1 \bar{C} X_2 X_3 \Delta \eta_2 \Delta \eta_3)_u - (\bar{U}_1 \bar{C} \eta_2 \Delta \eta_1 \Delta \eta_3 X_3 \frac{dX_2}{d\eta_1})_e$$

$$+ (\bar{U}_1 \bar{C} \eta_2 \Delta \eta_1 \Delta \eta_3 X_3 \frac{dX_2}{d\eta_1})_w - (\bar{U}_1 \bar{C} \eta_3 \Delta \eta_1 \Delta \eta_2 X_2 \frac{dX_3}{d\eta_1})_n +$$

$$(\bar{U}_1 \bar{C} \eta_3 \Delta \eta_1 \Delta \eta_2 X_2 \frac{dX_3}{d\eta_1})_s - (\bar{U}_1 \bar{C} \Delta \eta_1 \Delta \eta_2 X_2 \frac{dX_s^1}{d\eta_1})_n +$$

$$(\bar{U}_1 \bar{C} \Delta \eta_1 \Delta \eta_2 X_2 \frac{dX_s^1}{d\eta_1})_s + (\bar{U}_3 \bar{C} \Delta \eta_1 \Delta \eta_2 X_2)_n - (\bar{U}_3 \bar{C} \Delta \eta_1 \Delta \eta_2 X_2)_s -$$

$$(K_2 \frac{C_E - C_P}{\Delta \eta_2} \frac{\Delta \eta_1 \Delta \eta_3 X_3}{X_2})_e + (K_2 \frac{C_P - C_w}{\Delta \eta_2} \frac{\Delta \eta_1 \Delta \eta_3 X_3}{X_2})_w -$$

$$(K_s \frac{C_N - C_P}{\Delta \eta_3} \frac{\Delta \eta_1 \Delta \eta_2 X_2}{X_3})_n + (K_3 \frac{C_P - C_s}{\Delta \eta_3} \frac{\Delta \eta_1 \Delta \eta_2 X_2}{X_3})_s = S_P C_P + S_u$$

(D1.2)

Here the bracketed terms are averages over the boundaries (denoted by the suffix) in question. In equation (D1.2) a linear variation of $\bar{C}$ between nodes has been assumed in order to transform the diffusion terms to finite-difference form (note that when upwind differencing is employed diffusion is neglected).

(D1.2) can be simplified to:

$$\begin{aligned} & C_d G_d A_d - C_u G_u A_u - C_e G_e A_e + C_w G_w A_w + C_n G_n A_n - C_s G_s A_s - \\ & \frac{1}{Pe_e} G_e A_e (C_E - C_P) + \frac{1}{Pe_w} G_w A_w (C_P - C_W) - \frac{1}{Pe_n} G_n A_n (C_N - C_P) + \\ & \frac{1}{Pe_s} (C_P - C_S) = S_P C_P + S_U \end{aligned} \quad (D1.3)$$

where

$$G_d = (\bar{U}_1)_d \quad (D1.4.a)$$

$$G_e = (\bar{U}_1 \eta_2 \frac{dX_2}{d\eta_1})_e \quad (D1.4.b)$$

$$G_n = (\bar{U}_3 - \bar{U}_1 \frac{dX_1}{d\eta_1} - \bar{U}_{13} \frac{dX_3}{d\eta_1})_n \quad (D1.4.c)$$

G_u , G_w and G_s have similar expressions as G_d , G_e and G_n but for the u, w and s boundaries respectively

$$A_d = (X_2 X_3 \Delta \eta_2 \Delta \eta_3)_d \quad (D1.5.a)$$

$$A_e = X_3 \Delta \eta_1 \Delta \eta_3 \quad (D1.5.b)$$

$$A_n = X_2 \Delta \eta_1 \Delta \eta_2 \quad (D1.5.c)$$

A_u , A_w and A_s again have similar expressions as A_d , A_e and A_n respectively.

$$Pe_e = \left(\frac{GX_2 \Delta \eta_2}{K_2} \right)_e \quad (D1.6.a)$$

$$Pe_n = \left(\frac{GX_3 \Delta \eta_3}{K_3} \right)_n \quad (D1.6.b)$$

Pe_w and Pe_s are similar to Pe_e and Pe_n respectively.

From the continuity equation we have

$$G_d A_d = G_u A_u + G_s A_s - G_n A_n + G_e A_e - G_w A_w \quad (D1.7)$$

and by applying upwind differencing in the streamwise direction and central differencing elsewhere there results after rearrangement of equation (D1.3)

$$\begin{aligned} & C_p (G_u A_u - G_w A_w + G_e A_e + G_s A_s - G_n A_n - G_e A_e / 2 + G_w A_w / 2 \\ & + G_n A_n / 2 - G_s A_s / 2 + (GA/Pe)_e + (Ga/Pe)_w + (GA/Pe)_s + S_p \\ & = G_u A_u C_u + G_e A_e (\frac{1}{2} + 1/Pe_e) C_E + G_w A_w (-\frac{1}{2} + 1/Pe_w) C_W + \\ & G_n A_n (-\frac{1}{2} + 1/Pe_n) C_N + G_s A_s (\frac{1}{2} - 1/Pe_s) C_S + S_U \dots \end{aligned} \quad (D1.8)$$

which can be rewritten as:

$$\begin{aligned} C_p (a_u + a_w + a_e + a_s + a_n - S_p) & = a_u C_U + a_w C_W + a_e C_E \\ & + a_s C_S + a_n C_N + S_U \end{aligned} \quad (D1.9)$$

where

$$a_u = G_u A_u \quad (D1.10.a)$$

$$a_w = G_w A_w (-\frac{1}{2} + 1/Pe_w) \quad (D1.10.b)$$

$$a_e = G_e A_e (\frac{1}{2} + 1/Pe_l) \quad (D1.10.c)$$

$$a_n = G_n A_n (-\frac{1}{2} + 1/Pe_n) \quad (D1.10.d)$$

$$a_s = G_s A_s (\frac{1}{2} + 1/Pe_s) \quad (D1.10.e)$$

Only cases where Pe_s and Pe_n are greater than 2 will be derived here (other cases are similarly derived). In that case diffusion at the n and s boundaries are neglected and C_n and C_s are set equal to:

$$C_n = C_p, C_s = C_s$$

With these conditions inserted equation (D1.3) reduces, after applying the continuity equation, to

$$\begin{aligned} C_p (G_u A_u - G_w A_w + G_e A_e - G_n A_n + G_s A_s - G_e A_e / s + G_w A_w / 2 \\ + G_n A_n + (GA/Pe)_e + (GA/Pe)_w - S_p) = G_u A_u C_u + G_e A_e (\frac{1}{2} - 1/Pe)_e C_E \\ + G_w A_w (-\frac{1}{2} + 1/Pe_w) C_W + G_s A_s C_S + S_U \end{aligned} \quad (D1.11)$$

or

$$C_p (a_u + a_e + a_w + a_s - S_p) = a_u C_u + a_e C_E + a_w C_W + a_s C_S + S_U \quad (D1.12)$$

where

$$a_s = G_s A_s \quad (D1.13)$$

and a_w and a_e having the previous values as in (D1.10.b) and (D1.10.c) respectively.

APPENDIX D2

THE FUNCTIONS F_1 , F_2 AND F_3 APPEARING WHEN EMPLOYING
NEWTON-RAPHSON METHOD OF SOLUTION

The functions F_1 , F_2 and F_3 appearing in equations
(4.40), (4.41) and (4.42) have the following forms:-

$$F_1(\bar{u}_1\bar{u}_3, \bar{u}_3, Pr_t) = \frac{\bar{u}_3^2 Pr_t A_2}{\bar{k}} + Rt Pr_t \frac{\bar{u}_3^2}{\bar{k}} - Rt B \frac{\bar{u}_3^2}{\bar{k}} - \frac{2Rt(Pr_t A_5 - BA_6)}{3} - \frac{2Pr_t A_1}{3} \quad (D2.1)$$

$$F_2(\bar{u}_1\bar{u}_3, \bar{u}_3^2, Pr_t) = 0.5\bar{u}_1\bar{u}_3 Rt^2 (Pr_t - B)^2 + Rt\bar{u}_1\bar{u}_3 Pr_t (0.5(A_7 - 1) + c_{ic})(Pr_t - B) + \bar{u}_1\bar{u}_3 Pr_t^2 (A_3 A_7 - 0.5Rt^2 k \frac{\bar{u}_3^2 A_8}{\bar{u}_1\bar{u}_3} + BRt^2 \frac{k^2}{\bar{u}_1\bar{u}_3} A_9) + 0.5BRt^2 Pr_t k \frac{u_3^2}{\bar{u}_1\bar{u}_3} A_8 - kRt Pr_t^2 \frac{\bar{u}_3^2}{\bar{u}_1\bar{u}_3} A_8 A_3 + \frac{k^2}{\bar{u}_1\bar{u}_3} Pr_t BRt^2 A_4 A_9 \quad (D2.2)$$

$$F_3(\bar{u}_1\bar{u}_3, \bar{u}_3^2, Pr_t) = Pr_t^3 \frac{\bar{u}_3^2 A_3 A_7}{\bar{k}} + Rt Pr_t^2 \frac{\bar{u}_3^2}{\bar{k}} (Pr_t - B)(A_3 + 0.5A_7) + 0.5Rt^2 Pr_t \frac{\bar{u}_3^2 M}{\bar{k}} - Rt Pr_t^2 BA_7 A_3 A_{10} c_\theta - Rt^2 B Pr_t (A_3 + 0.5A_7) (Pr_t - B) c_\theta A_{10} - 0.5Rt^3 M c_\theta BA_{10} + Rt B Pr_t^2 A_{11} A_9 + 0.5Rt^2 Pr_t B (Pr_t - B) A_9 - Pr_t^2 \frac{\bar{u}_3^2 A_{11} A_3 A_8}{\bar{k}} - 0.5Rt Pr_t \frac{\bar{u}_3^2}{\bar{k}} (Pr_t - B)(A_3 + A_{11}) A_8 - 0.25Rt^2 M \frac{\bar{u}_3^2 A_8}{\bar{k}} - Rt Pr_t BA_{11} A_4 A_9 - 0.5Rt^2 B (Pr_t - B) A_4 A_9 \quad (D2.3)$$

where:

$$B = \frac{g\bar{\theta}_{,3}}{\theta_m \bar{U}_{1,3}^2}$$

$$M = Pr_t^2 - 2Pr_t^2 B - B^2$$

$$Pr = -\overline{u_1 u_3} \bar{U}_{1,3} / \varepsilon$$

$$A_1 = c_1 - 1$$

$$A_2 = c_1 - 1 + 2c_2' f(1/x_3)$$

$$A_3 = c_{1c} - 0.5$$

$$A_4 = c_{2c} - 1$$

$$A_5 = c_2 - 2c_2 c_2' f(1/x_3)$$

$$A_6 = 3 - 2c_3 + 4c_3 c_3' f(1/x_3)$$

$$A_7 = c_1 - 1 + 1.5c_1' f(1/x_3)$$

$$A_8 = 1 - c_2 + 1.5c_2 c_2' f(1/x_3)$$

$$A_9 = 1 - c_3 + 1.5c_3 c_3' f(1/x_3)$$

$$A_{10} = 1 - c_{3c} - c_{3c} c_{3c}' f(1/x_3)$$

$$A_{11} = c_{1c} - 0.5 + c_1' f(1/x_3)$$

APPENDIX E1

ON THE SIMILARITY OF NORMALISED CONCENTRATION PROFILES IN A TWO DIMENSIONAL FIELD

For a line source placed at ground level, equation (4.7) could be re-written as

$$x_3 \bar{U}_1 \frac{\partial \bar{C}}{\partial \eta_1} - \eta_3 \bar{U}_1 \frac{\partial C}{\partial \eta_3} \frac{dx_3}{d\eta_1} + \bar{U}_3 \frac{\partial \bar{C}}{\partial \eta_3} = \frac{1}{x_3} \frac{\partial}{\partial \eta_3} K_3 \frac{\partial \bar{C}}{\partial \eta_3} \quad (E1.1)$$

By normalising equation (E1.1) by dividing through by $C_m U_o$, where U_o is some velocity scale, and noting that

$$\frac{\partial \bar{C}/C_m}{\partial \eta_1} = -\frac{\bar{C}}{C_m^2} \frac{\partial C_m}{\partial \eta_1} + \frac{1}{C_m} \frac{\partial \bar{C}}{\partial \eta_1} \quad (E1.2)$$

then if $\bar{C}/C_m$ is independent of η_1 and by substituting (E1.2) into (E1.1) we get:

$$\begin{aligned} x_3 \frac{\bar{U}_1}{C_m U_o} h(\eta_3) \frac{dC_m}{d\eta_1} - \frac{\eta_3 \bar{U}_1}{U_o} \frac{\partial h(\eta_3)}{\partial \eta_3} \frac{dx_3}{d\eta_1} + \frac{\bar{U}_3}{U_o} \frac{\partial h(\eta_3)}{\partial \eta_3} = \\ \frac{1}{U_o x_3} \frac{\partial}{\partial \eta_3} K_3 \frac{\partial h(\eta_3)}{\partial \eta_3} \end{aligned} \quad (E1.3)$$

where $h(\eta_3) = \bar{C}/C_m$.

Now if h is to be a function of only η_3 (as is assumed) then all terms in (E1.3) must be either constant or independent of any parameters other than η_3 .

In boundary layer flows over a flat plate no velocity

scale (U_0) exists that will render $\bar{U}_1/U_0$ independent of η_1 ; however $(U_1 - U_{1\infty})/U_0$ could be independent of downstream distance (though it will be a function of x_3/δ as noted in Hinze (1975)) if U_0 is taken as u_* . In that case

$$\frac{\bar{U}_1 - U_{1\infty}}{u_*} = f(x_3/\delta) \quad (\text{El.4})$$

where f is some function of x_3/δ . By manipulating the continuity equation and using (El.4) we can write

$$\begin{aligned} \frac{\bar{U}_3}{u_*} &= \left(\frac{du_* \delta}{d\eta_1} \frac{1}{u_*} + \frac{d\delta}{d\eta_1} \right) \int f\left(\frac{x_3}{\delta}\right) d\left(\frac{x_3}{\delta}\right) + \frac{d\delta}{d\eta_1} \frac{x_3}{\delta} f\left(\frac{x_3}{\delta}\right) - \\ &\quad \frac{\delta}{u_*} \frac{x_3}{\delta} \frac{dU_{1\infty}}{d\eta_1} \end{aligned} \quad (\text{El.5})$$

By employing experimental data that describe the variation of u_* and δ with η_1 it can be shown that $\bar{U}_3/u_*$ will be a weak function of η_1 hence

$$\frac{\bar{U}_3}{u_*} \approx g\left(\frac{x_3}{\delta}\right) \quad (\text{El.6})$$

where g is another function of x_3/δ .

Equations (El.4) and (El.6) could be re-written as:

$$\frac{U_1 - U_{1\infty}}{u_*} = f\left(\frac{x_3}{X_3^\alpha}\right) \quad (\text{El.7})$$

$$\frac{\bar{U}_3}{u_*} = g\left(\frac{x_3}{X_3^\alpha}\right) \quad (\text{El.8})$$

where $\alpha = X_3/\delta$.

Substituting (E1.7) and (E1.8) into (E1.3) after some manipulations we get*

$$\begin{aligned} & \left[\frac{U_{1\infty}}{u_*} - f(\eta_3 \alpha) \right] \left[\frac{h(\eta_3)}{C_m} X_3 \frac{\partial C_m}{\partial \eta_1} + \eta_3 \frac{\partial h(\eta_3)}{\partial \eta_3} \frac{dX}{d\eta_1} \right] + g(\eta_3 \alpha) \frac{\partial h(\eta_3)}{\partial \eta_3} \\ & = \frac{\partial}{\partial \eta_3} \bar{K}_3(\eta_3 \alpha) \frac{\partial h(\eta_3)}{\partial \eta_3} \end{aligned} \quad (E1.9)$$

$$\text{where } \bar{K}_3(\eta_3 \alpha) = \frac{K_3}{u_* \delta} \frac{\delta}{X_3}$$

From Schlichting (1968)

$$\frac{u_*}{U_{1\infty}} = 0.172 \frac{(U_{\infty} \eta_1)^{-1/10}}{\nu} \quad (E1.10)$$

and from relations (6.4) and (6.5)

$$\frac{X_3 dC_m}{C_m d\eta_1} \propto \eta_1^{-0.2} \quad (E1.11)$$

$$\frac{dX_3}{d\eta_1} \propto \eta_1^{-0.2} \quad (E1.12)$$

*Note that X_3 can take an arbitrary value; here it is taken equal to λ_3 .

†By employing the mixing length hypothesis $K_3 = u_* \kappa X_3 / Sc_t$ and assuming a constant Schmidt number Sc_t .

Substituting (E1.10), (E1.11) and (E1.12) we finally get

$$\begin{aligned} & \{a(\eta_1)^{-0.1} - f(\eta_3\alpha)\} \{bh(\eta_3)\eta_1^{-0.2} + d\eta_3 \frac{\partial h(\eta_3)}{\partial \eta_3} \eta_1^{-0.2}\} \\ & + g(\eta_3\alpha) \frac{\partial h(\eta_3)}{\partial \eta_3} = \frac{\partial}{\partial \eta_3} \tilde{\kappa}_3(\eta_3\alpha) \frac{\partial h(\eta_3)}{\partial \eta_3} \end{aligned} \quad (E1.13)$$

where a , b and d are constants (assuming $\bar{U}_{1\infty}$ is constant). From the direct appearance of η_1 in equation (E1.13) and because α depends on η_1 it is obvious that $h(\eta_3)$ cannot be entirely independent of η_1 .

Table 3.1 Turbulence model constants

Model constant	c_1	c_2	c_3	c'_1	c'_2	c'_3	c_{1c}	c_{2c}	c_{3c}	c'_{1c}
Value	1.8	0.6	0.5	0.5	0.3	0	3	0.33	0.33	0.5
Model constant	c'_{2c}	c'_{3c}	c_θ	a_3	a'	$c_{\epsilon 1}$	$c_{\epsilon 2}$	$c_{\epsilon 3}$	c_ϵ	c_s
Value	0	0	1.6	0.55	0.9	1.44	1.9	1.55	0.17	0.25

Table 4.1
Definition of P^Φ and Γ_3^Φ for different variables
in ξ_1, ξ_2, ξ_3 coordinates

	P^Φ	Γ_3^Φ
$\bar{U}_1$	0	$-\delta \bar{u}_1 \bar{u}_3 / \partial U_1 / \partial \xi_3$
$\bar{\theta}$	0	$-\delta \bar{u}_3 \bar{\theta} / \partial \theta / \partial \xi_3$
k	$\frac{-l \bar{u}_1 \bar{u}_3}{\delta} \frac{\partial U_1}{\partial \xi_3} (1-Rf)$ -ε	$c_s \frac{k \bar{u}_3^2}{\epsilon}$
ε	$-c_{\epsilon 1} \frac{l \bar{u}_1 \bar{u}_3}{\delta} \frac{\partial U_1}{\partial \xi_3} \frac{\epsilon}{k}$ $-c_{\epsilon 2} \frac{\epsilon^2}{k}$ $+c_{\epsilon 3} \beta_3 \bar{u}_3 \frac{\partial \bar{u}_1}{\partial \xi_3}$	$c_\epsilon \frac{k \bar{u}_3^2}{\epsilon}$

TABLE 5.1 - MEASURED CONCENTRATION IN VPPM FOR GROUND RELEASES* (WITH SMOOTH SURFACE)

(i) $x_1 = 0.5$ m

$x_2 \backslash x_3$	0.65	1.69	2.74	3.78	4.8	5.8
0	2354	1433	631	247	85.3	60
0.83	2132	1347	605	238	85	59
1.83	1535	1023	477	213	68	37
2.8	892	631	321	136	48	22
4.11	278	216	127	59.7	28.4	17
0.5	108	108	59.7	28.4	17	-
-0.8	2474	1501	708	281	110	42.65
-1.8	2115	1296	597	230	85.3	34
-3.0	1228	759	409	170	59.2	-
-4.0	625	426	255	96	45.5	22
-5.2	204	125	91	45.5	19.9	-
-6.2	56.8	54	28.4	-	-	-

*Values of x_2 and x_3 are in centimetres

TABLE 5.1 - CONTINUED

(ii) $x_1 = 1$ m

$x_3 \backslash x_2$	0.65	1.95	3.25	4.53	5.81	7.06	8.32
0	955	688	412	218	99	48	25.5
0.8	853	662	418	236	122	56	27
1.8	756	571	372	207	99	45.5	-
2.8	557	455	284	167	82.4	39.8	25
4.0	483	298	193	122	65.4	34	-
5.5	183	161	117	72	38.5	21	-
7.0	80.5	84.4	67.38	38.5	26.25	16.61	-
-8.0	929	671	383	213	105	48.3	22.7
-1.6	881	634	372	199	102	48.3	28.44
-2.8	747	548	321	176	96.7	45.5	28.44
-4.3	548	366	233	122	65.41	65.41	36
-5.8	3.2	238	150.7	85.3	51.1	28	-
-7.5	151	122	98.88	53.3	35	23.6	-
-9.5	47	49	43.7	28.8		-	-

TABLE 5.1 - CONTINUED

(iii) $x_1 = 1.5$ m

$x_3 \backslash x_2$	0.65	2.15	3.65	5.13	6.59	8.04	9.51	11
0	477.7	372	270.15	162.1	99.5	56.8	39.1	17
1.3	423	349	253	159	96.68	56.8	30.4	-
2.8	335	276	208	145	84.8	48.1	26.2	-
4.5	206	194	147	96.25	62.22	37.6	22.22	-
6.5	115	99.75	80.5	56.8	38.5	26.2	437	-
-1.2	503	403	270	175	100	62.5	34	-
-2.5	460	375	273	182	116	68.2	34	-
-2	375	301	258	136	73.8	45.5	-	-
-6	253	246	210	127	55	47	28	-
-8	168	152	105	66	37.6	24.5	-	-
-11	50.7	50.7	48	30	17.5	-	-	-

TABLE 5.1 - CONTINUED

(iv) $x_1 = 2.5$ m

x_3 x_2	0.68	2.16	3.65	5.13	6.59	8.05	9.51	10.99	12.49	13.9
0	231	207	172	134	93.6	77	55	35	24.5	-
2	183	170	150	122	87	74	50.7	37.6	24.5	-
4	166	147	126	100	80	61.25	43.7	30.6	21.8	-
7	80.6	77	64.7	52	40.2	31.5	28	-	-	-
10	38	38	38	35	30	30	-	-	-	-
-2	246	21.7	180	136	103	75	51.7	34.4	-	-
-4	227	203	179	147	119	91	66.6	51	37.6	26
-6.5	163	159	131	113	90.1	70	54	37.6	24	-
-9.5	87	87	78.7	67	58	48	35	28.8	-	-
-12.5	47	45.6	43.7	35	32	26	23	17.5	-	-
-16	17	17	-	-	-	-	-	-	-	-

TABLE 5.2 - MEASURED CONCENTRATION IN VPPM FOR GROUND RELEASE (WITH CHANGE IN SURFACE ROUGHNESS)

(i) $x_1 = 1 \text{ m}$

$\begin{matrix} x_3 \\ x_2 \end{matrix}$	1.1	2.3	3.5	4.68	5.84	7.0	8.16	9.33	10.54
0	722	676	503	321	190	108	56.8	28.4	17
0.8	682	651	511	325	193	102	56.8	28.4	17
1.8	597	597	437	285	170	102	55.7	28.4	17
2.8	426	426	312	204	120	78	36.9	22.7	17
4	234	251	208	145	92.3	54.7	32.99	17.36	-
5.5	138.9	143	112	81.5	56.44	29.5	19.4	12.15	-
7	63.38	65.1	54.7	36.8	27.7	18.2	13.8	9.5	-
-0.8	764	709	540	341	266	171	52	22.7	17
-1.8	750	665	506	330	190	93	52	22.7	-
-2.8	716	660	497	315	187	96	53	24	-
-4	605	540	477	284	133	82	48	22.7	-
-5.5	324	267	204	127	69.3	34	22.7	11.3	-
-7.2	210	130	91	51	34	28.4	19	-	-
-9.25	85	56.8	34	25	-	-	-	-	-

TABLE 5.2 - CONTINUED

(ii) $x_1 = 1.5$ m

x_3 x_2	1.1	2.45	3.79	5.11	6.42	7.72	9.03	10.36	11.68
0	375	369	335	255	187	120	74	42.6	25.5
1.3	338	340	303	249	187	119	71	40.9	23
2.78	267	267	237	207	153	102	65	40	-
4.5	184	188	169	145	114	68	45	34	17
6.5	103	111	106	93.7	72	53	34	-	-
8.5	59	61	64	57.6	43.6	29.6	20	-	-
-1.3	386	369	327	261	184	127	73.93	42.6	-
-2.9	395	369	308	245	153	91	51	-	-
-5.5	321	290	255	193	127	82.4	48	28.4	-
-7.5	221	205	164	130	91	58	39	22.4	-
-9.5	130	131	104	77.9	62.5	36.52	24.3	17	-
-11	76	74.6	63.4	57	55	38.2	23.4	16.4	-

TABLE 5.2 - CONTINUED

(111) $x_1 = 2.5$ m

$x_3 \backslash x_2$	1.1	2.55	3.8	5.42	6.85	8.25	9.67	11.1	12.54	13.98
0	161	159	157	147	129	115	86	66	46	31
2	131	130	123	116	111	95	78.4	59.3	39.04	27.2
4	108	93	89.4	86	75.5	69.4	56.4	41.6	29.5	20
6	66.8	69.46	71	69.46	72	68.5	54.7	37.3	26.9	17.3
8	55.57	58.1	61.6	60.7	54.7	46	39.9	29.8	21.7	13.02
10	39	38.2	37.33	35.6	33	29.5	22.5	18.75	13.02	-
12	26.04	26.4	27.78	24.3	24.3	-	-	-	-	-
-2	159	158	160	147.9	131	115	94.6	75	50.3	35.6
-4	169	166	161	151	129.3	112	92.9	66	48.6	32
-6	146	145	132	118	101	92	72	56	38.2	27
-9	112	112	114	100	88.56	72	55.9	42.54	34.7	27
-12	93.77	85	86.8	80.7	65	55.5	46	34	22.5	17
-13.2	32.1	32.1	29.5	27.7	20.8	20	17.3	14.76	-	-

TABLE 5.3 - MEASURED CONCENTRATION IN VPPM FOR ELEVATED SOURCE

(i) $x_1 = 50$ cm

$x_3 \backslash x_2$	1.72	2.76	3.81	4.83	5.84	6.84	7.85	8.86	9.89
0	19.06	96.6	304	568	804.7	767.8	520.4	273	104
0.8	19	79.6	261	503	671	648	455	250	93
1.8	18.5	65.4	193	361	491	474	346	179	71
2.8	18.5	35.2	122	179	278	278	204	131	-
4	-	17.5	45.5	77.8	112.8	115	96	57.7	26
5.22	-	8.75	18.3	27.1	35	35	23.6	15.7	-
-0.8	25.5	93	307	591	819	764	534	312	127
-1.8	22.75	93.8	262	537	716	655	460	255	102
-2.8	19.9	76.7	216	386	500	452	290	162	65
-4	11.9	40.95	108	204	266	234	164	85.3	-
-5.5	5.25	14	43.4	61.3	82.2	73.5	49.8	28.8	-

TABLE 5.3 - CONTINUED

(ii) $x_1 = 1$ m

$x_2 \backslash x_3$	0.65	1.7	2.75	3.79	4.82	5.84	6.86	7.85	8.86	9.88	10.85	11.97
0	56.87	87.45	146	188.8	250	273	275.8	254	193.3	133.65	85.3	11.3
1	50	76	132	187	229	258	253	223	189	149	98	-
2	41.6	71	121	171	216	229	217	189	147	100	63.3	-
3.5	29.8	43	60.7	85.48	105	108	110	95.5	74.6	58.1	38	-
5	13.89	24.7	34.7	59.4	84	90.3	90.3	78.1	65	50	34	-
6.5	11.29	15.98	27.8	38.6	55.5	64.2	59.9	55.57	43.4	34.7	26.05	-
-1	53	84	144	181	258	284	286	269	225	180	107	58
-2.2	57.3	93.7	147	199	248	274	254	222	189	126	74.6	50
-3.7	45.1	75	131	196	229	250	246	187	145	108	60	-
-5.5	34.7	52	92.04	128	136	153	153	125	106	75	41	-
-7	16.4	28.65	37.3	57.3	64.25	71.2	67	56.44	53.8	48.63	32	-

TABLE 5.3 - CONTINUED

(iii) $x_1 = 1.5$ m

$x_3 \backslash x_2$	0.65	2.06	3.46	4.84	6.21	7.56	8.93	10.3	11.69	13.06	14.45	15.85
0	83.3	97.2	119	151	159.8	161	130	121.5	93.77	54.7	32.12	17.36
1.5	78.4	100	118	145	148	147	127	96.3	69.1	57	38.55	-
3	46	62.8	81.62	98.12	102.4	101	95.5	65.1	45.1	32	18.2	-
4.5	31	41.6	59.9	66.86	71.2	76.4	62.5	60	45	30.4	-	-
6.5	19.9	26	34.7	43.4	46.9	43.4	39.1	33	21.2	-	-	-
-1.5	78	107	126	158	164	164	147	130	93.8	69.1	42	-
-3	78.1	109	132	158	164	170	155	128.5	92	60	38	-
-4.5	78.1	95	126.8	145.8	151.1	144	123	102	80.75	53.48	32.16	-
-6.5	64.25	78	92	108	118	115	109	86.8	72.9	50.36	33	-
-8.5	35.6	40.8	48.45	58.7	60.8	58.3	48.6	41.3	29.5	20.8	13.9	-

TABLE 5.3 - CONTINUED

(iv) $x_1 = 2$ m

$\begin{matrix} x_3 \\ x_2 \end{matrix}$	0.65	2.25	3.85	5.42	6.98	8.59	10.12	11.72	13.3	14.9	16.5
0	95	102	116.35	123	117	111	89.43	84.2	46.9	27.7	-
1.5	76.4	76.4	90.3	99.8	110	111	93	76.4	55.5	33.3	24
3	61	66	81.6	90.3	95.6	87.75	80.75	66.3	47.2	36.4	-
5	48.9	52.1	61.65	65.124	70.3	66.86	54.7	47.75	32.12	30.4	19
7.3	30.39	37.85	48.6	53.83	58.17	56.44	49	38.2	26	19.97	13
9	19.1	24.3	29.5	33	34.7	34.7	33	27.8	20	-	-
-1.5	106	113	122	126	121	109	87.7	71.2	48	31	22.5
-3	98	101	112	113	115	107.6	91.1	70.85	87.3	41	-
-5	72	80.75	92	92.9	92	90.3	79	69.4	51.23	37.3	-
-7	64.6	68	80.75	84.22	83.3	79.8	66.33	57.3	45.1	32.1	20.8
-9.5	32.22	38.2	52.1	57.3	55.57	60.7	52.1	43.76	30.4	21.7	-
-12	19.1	23	24.66	30.4	32.12	32.12	27.8	22.57	15.63	13.71	-

Table 6.1 Running conditions for the atmospheric
predictions

Stability category	$U_{1\infty}$ (m/s)	δ^* (m)	H (W/m ²)	x_0 (m)
D-E	8	500	-9.5	0.1
D	8	500	0	0.1
B-C	8	600	140	0.1
B	8	750	320	0.1

* δ here is the boundary layer thickness specified
5000m upstream of the point of pollutant injection.

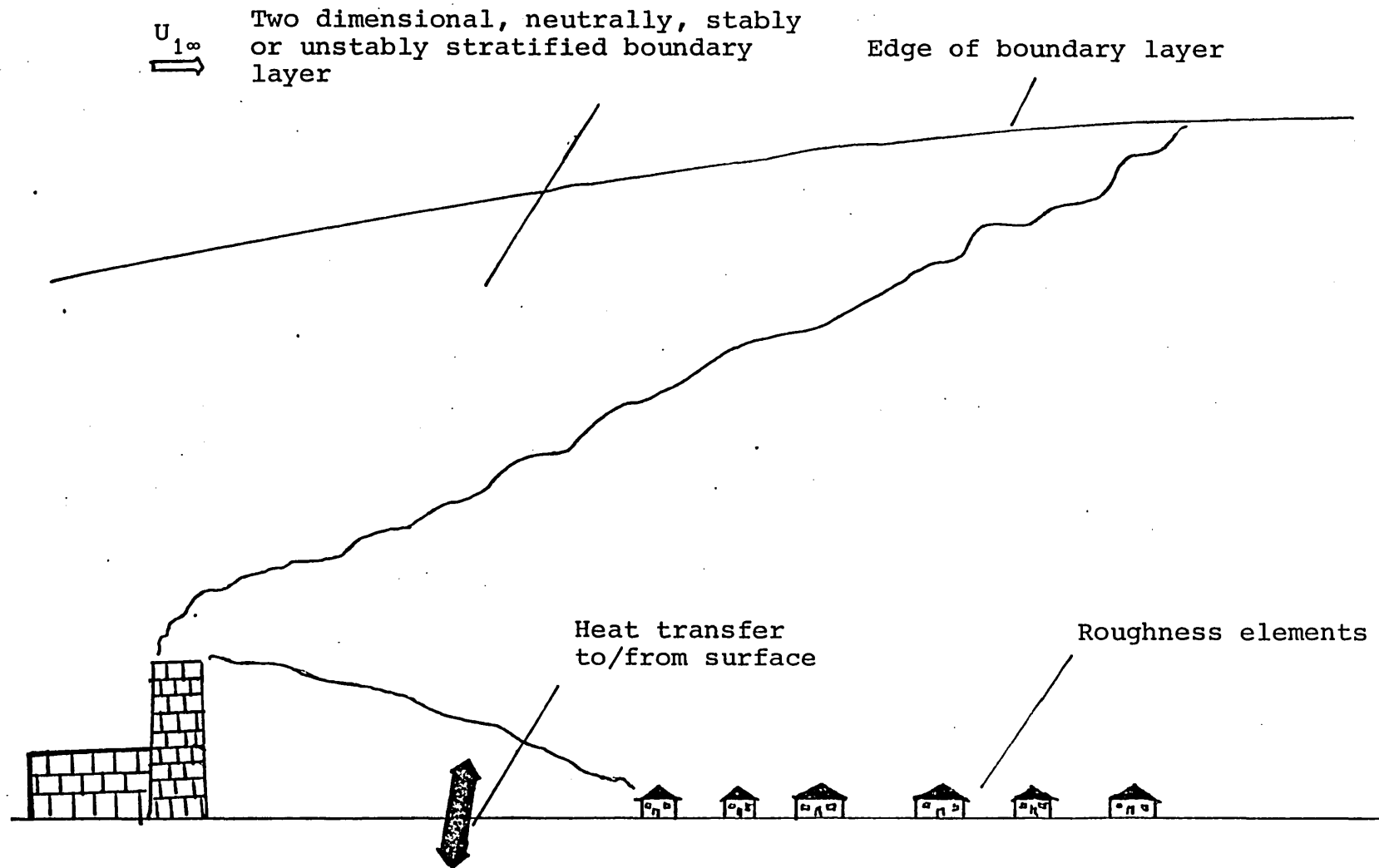


Figure 1.1 Schematic diagram of situation to be predicted

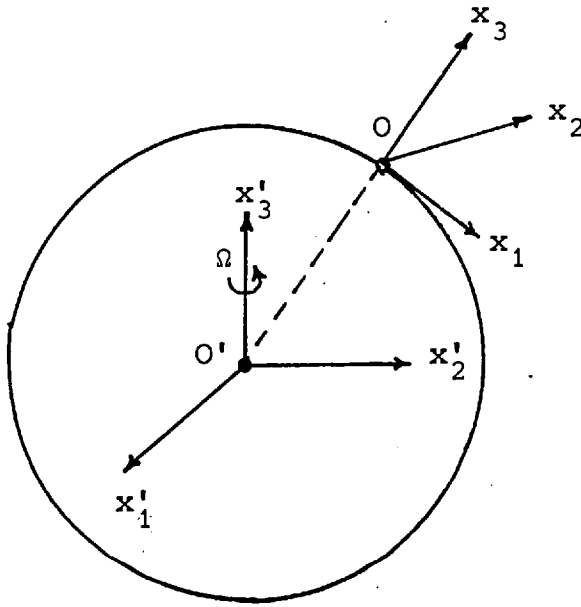


Figure 2.1 Diagram showing the two coordinate systems $Ox_1x_2x_3$ and $O'x'_1x'_2x'_3$

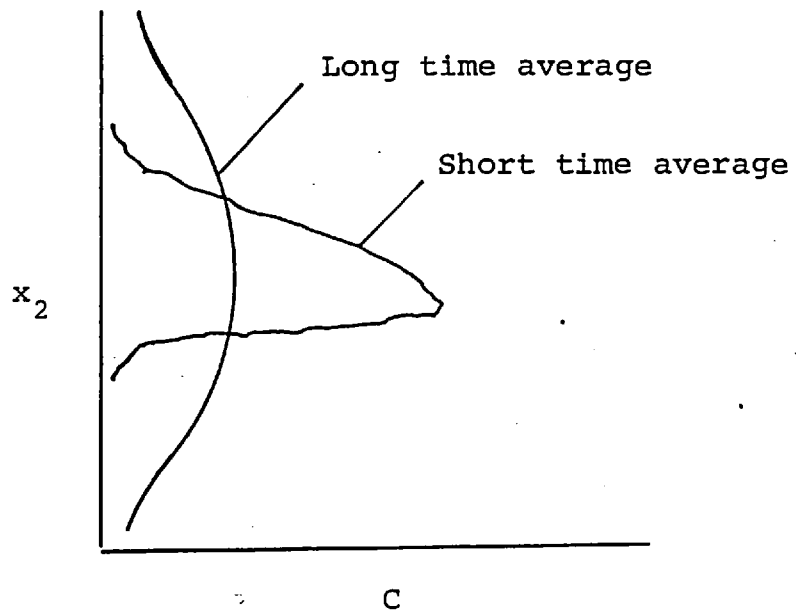


Figure 2.2 Schematic diagram of effect of averaging time on concentration

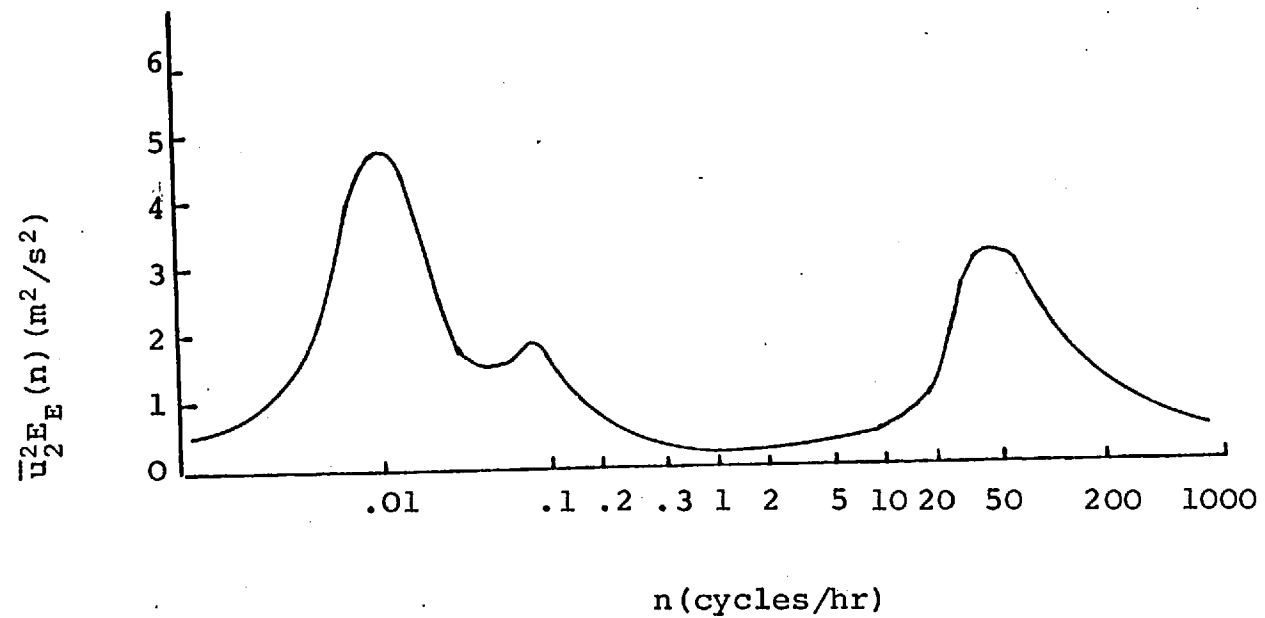


Figure 2.3 Horizontal wind speed spectrum of Brookhaven National Laboratory
(Van-Der-Hoven (1957))

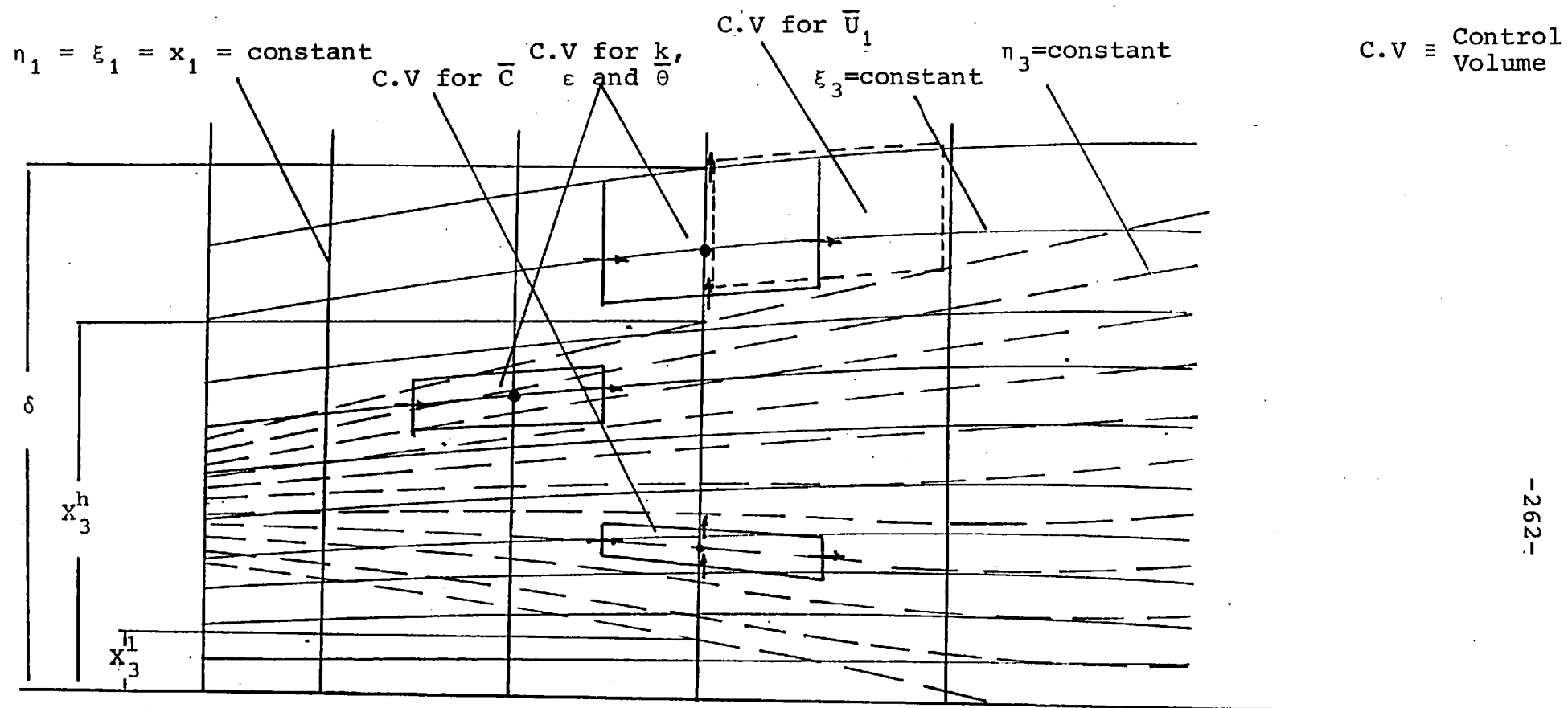


Figure 4.1a View of the two calculation grids in the x_1x_3 plane

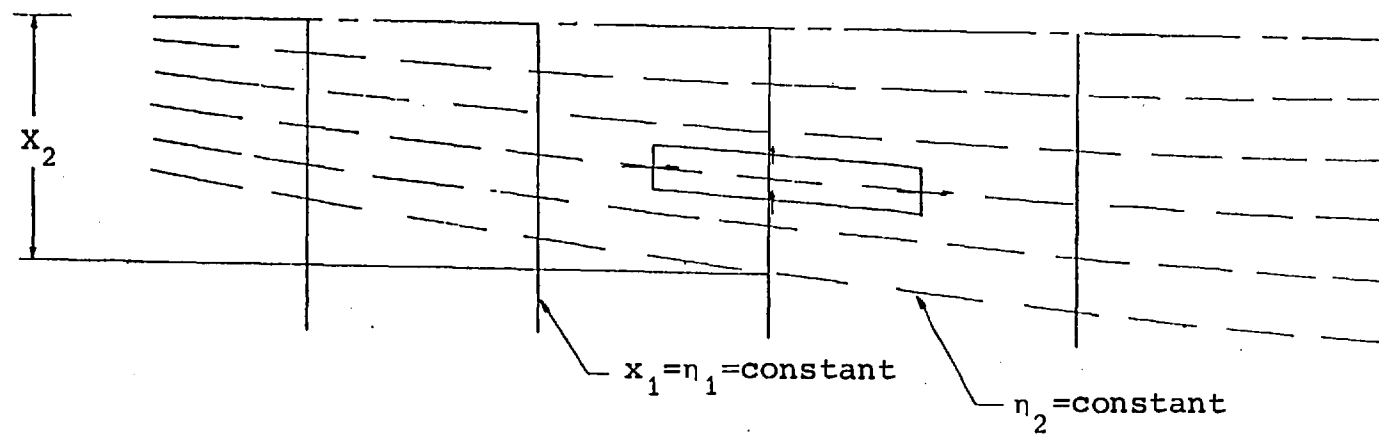


Figure 4.1b Concentration grid in x_1 - x_2 plane

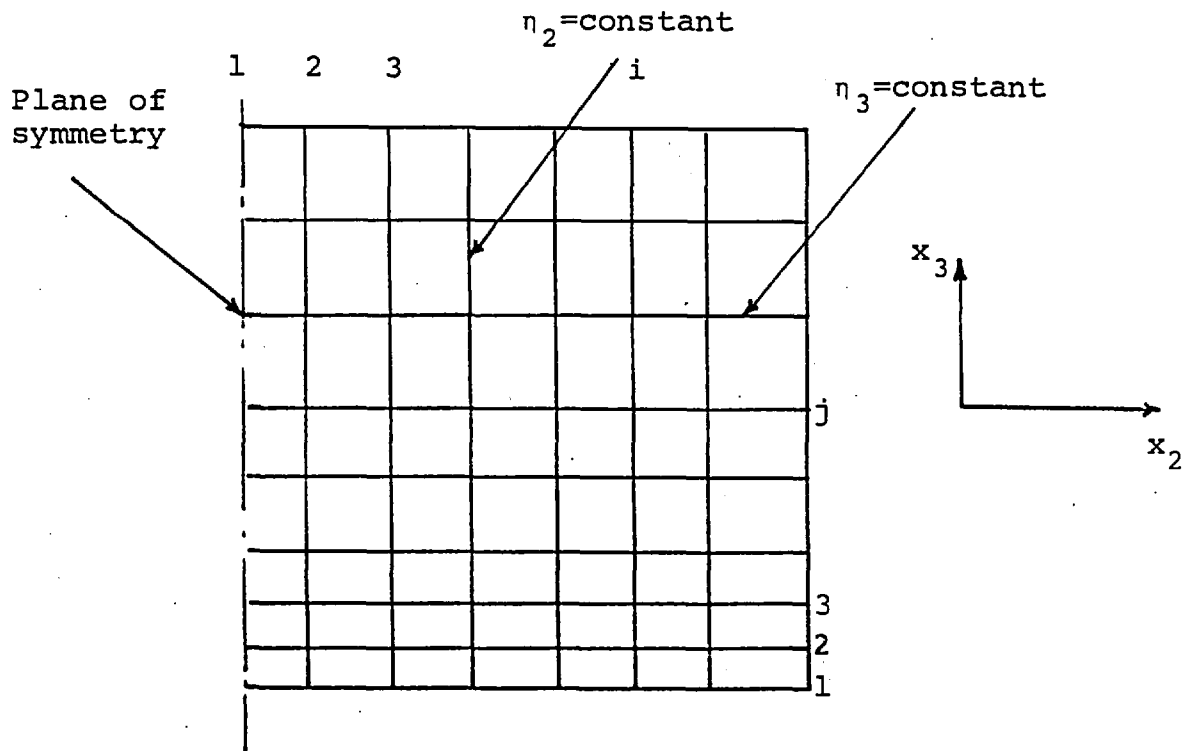


Figure 4.2 Concentration grid in x_2 - x_3 plane

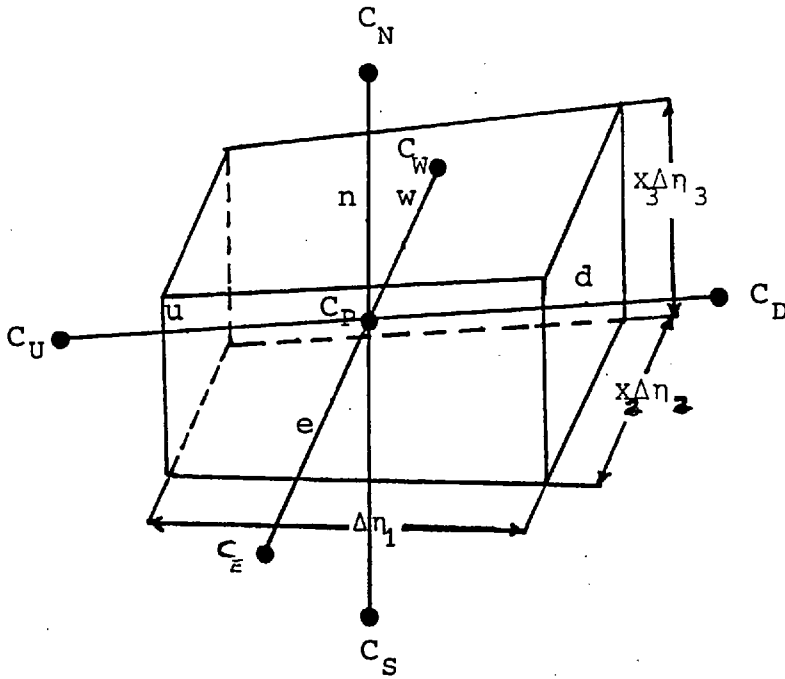


Figure 4.3 Micro-control volume for concentration grid

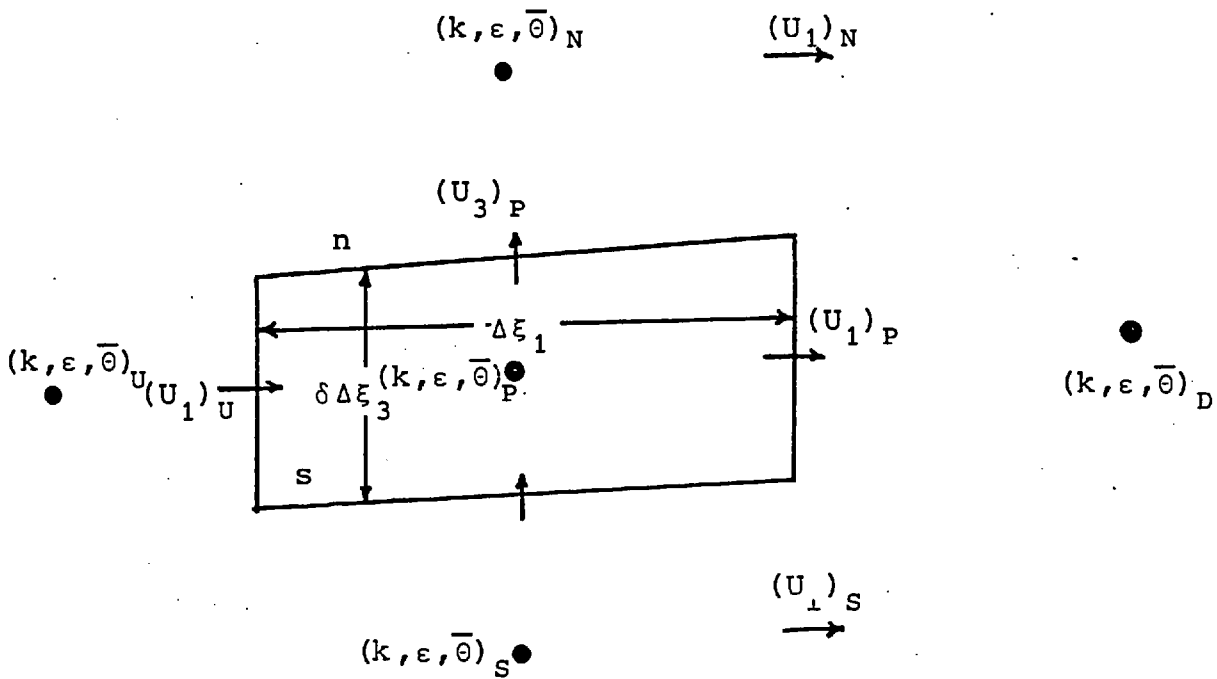


Figure 4.4 Micro-control volume for hydrodynamic grid

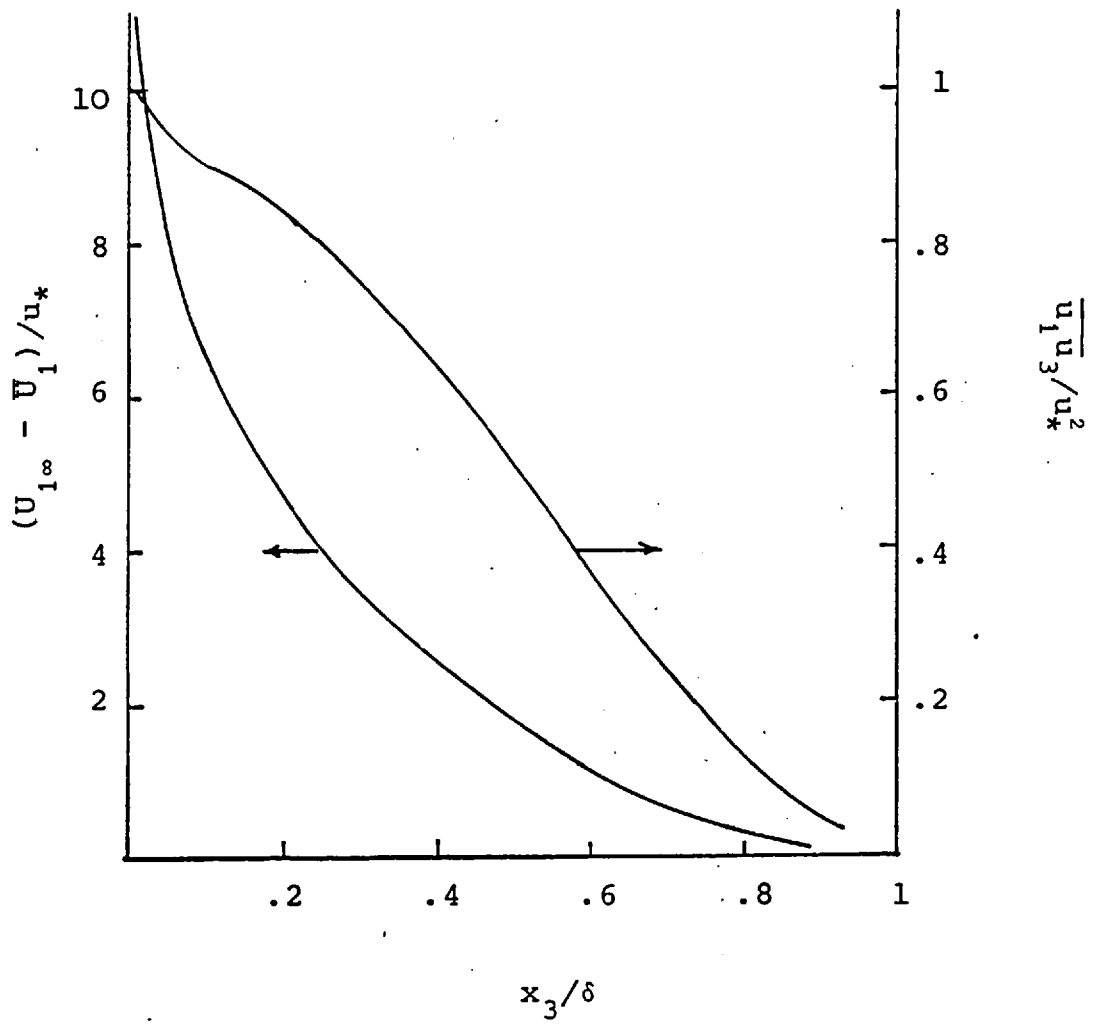


Figure 4.5 Normalised mean velocity and turbulent shear stress profiles

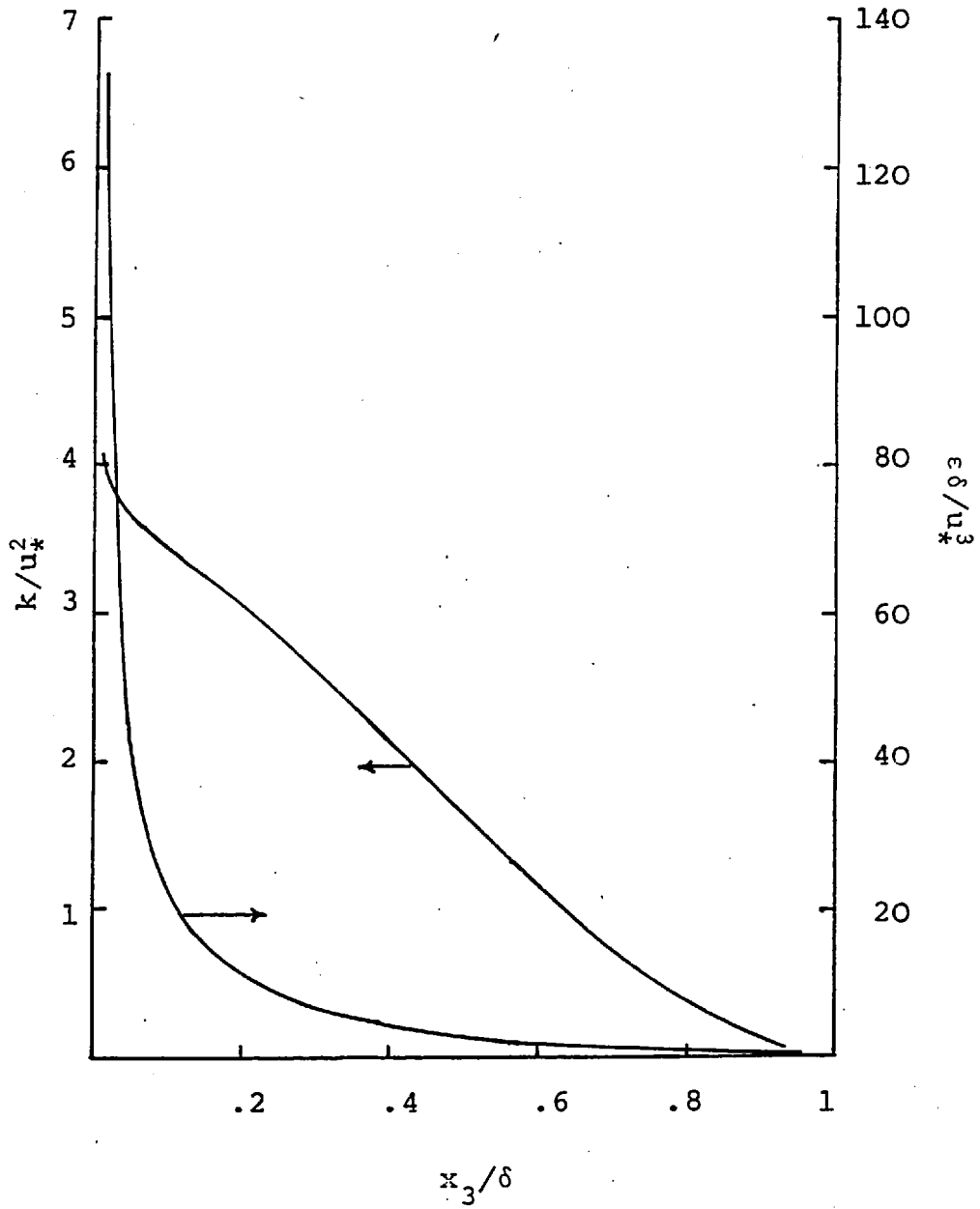


Figure 4.6 Normalised turbulence kinetic energy and dissipation rate profiles

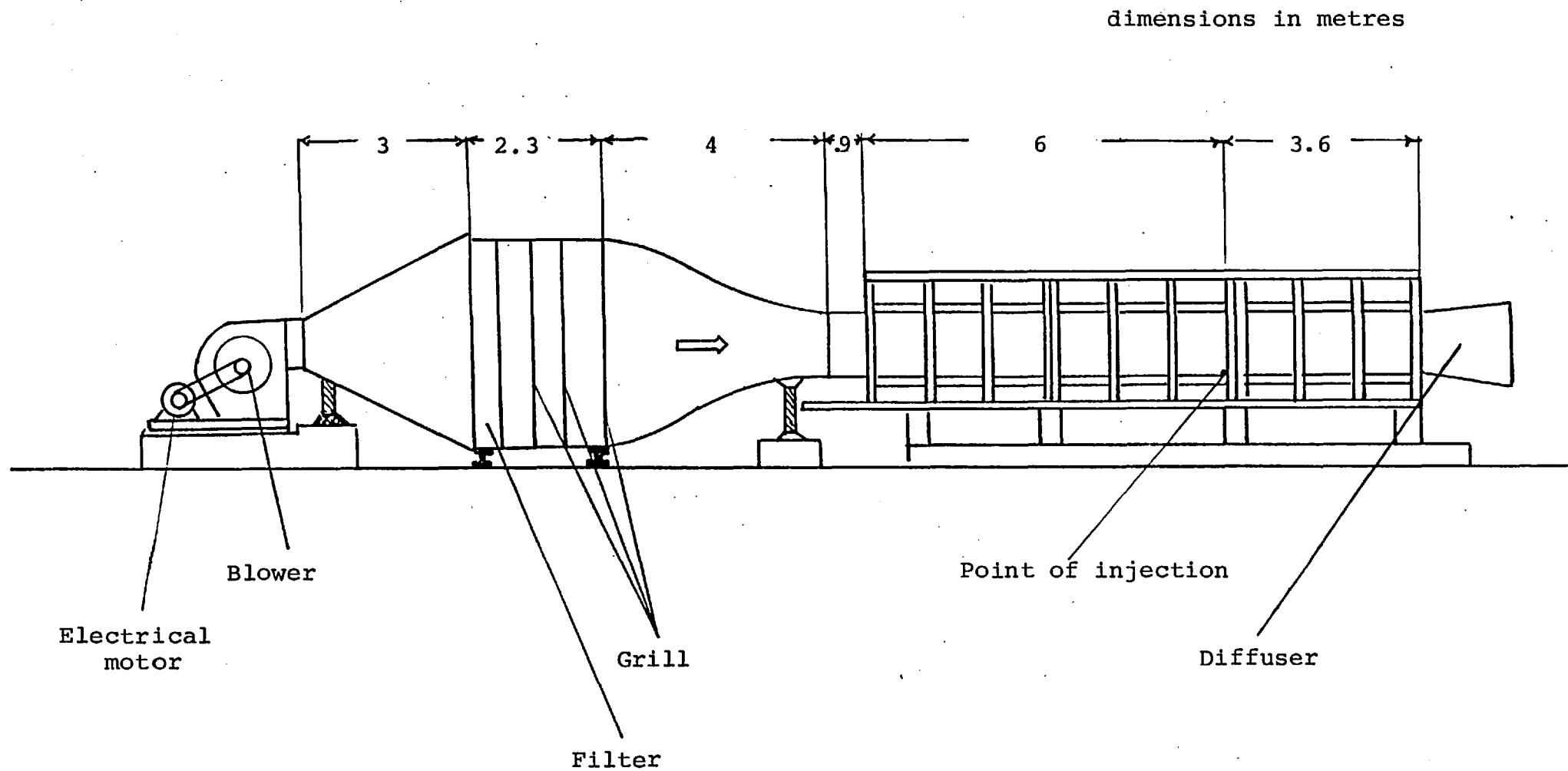


Figure 5.1 General view of wind tunnel

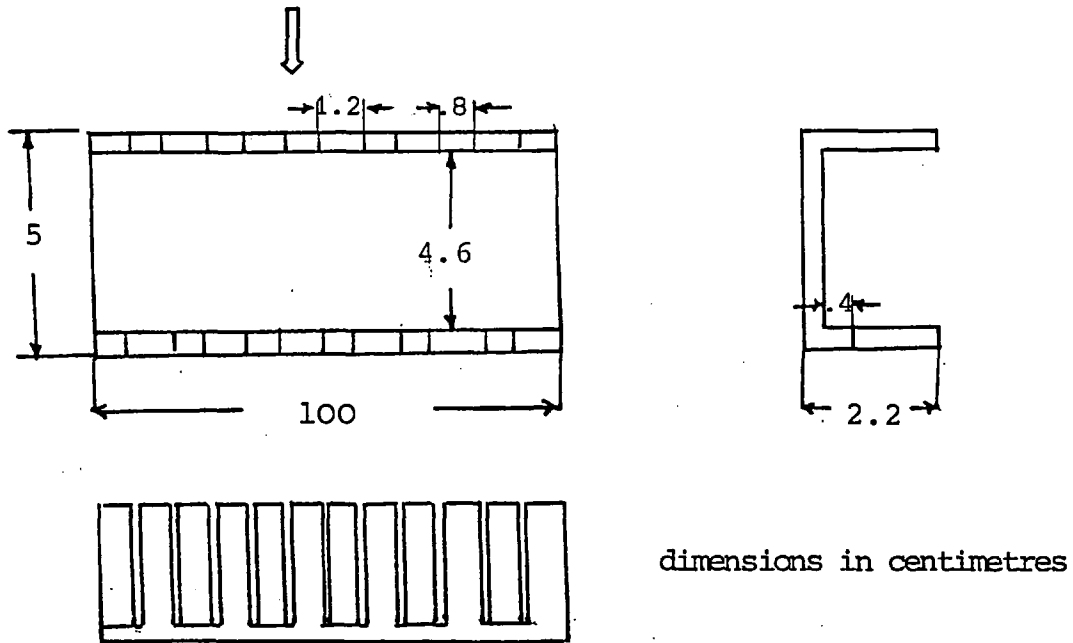


Figure 5.2 Three views of tripping roughness element

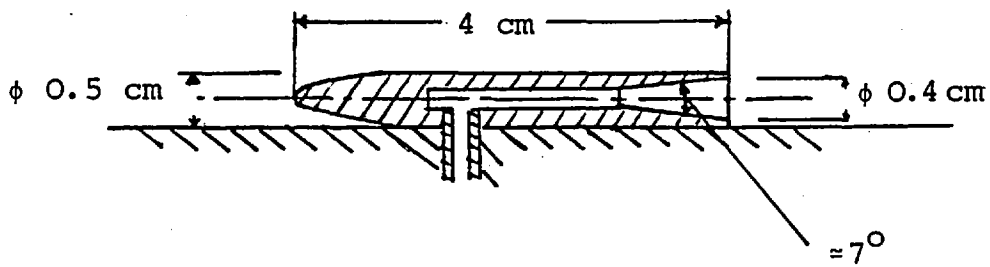


Figure 5.3 Ethane injection tube

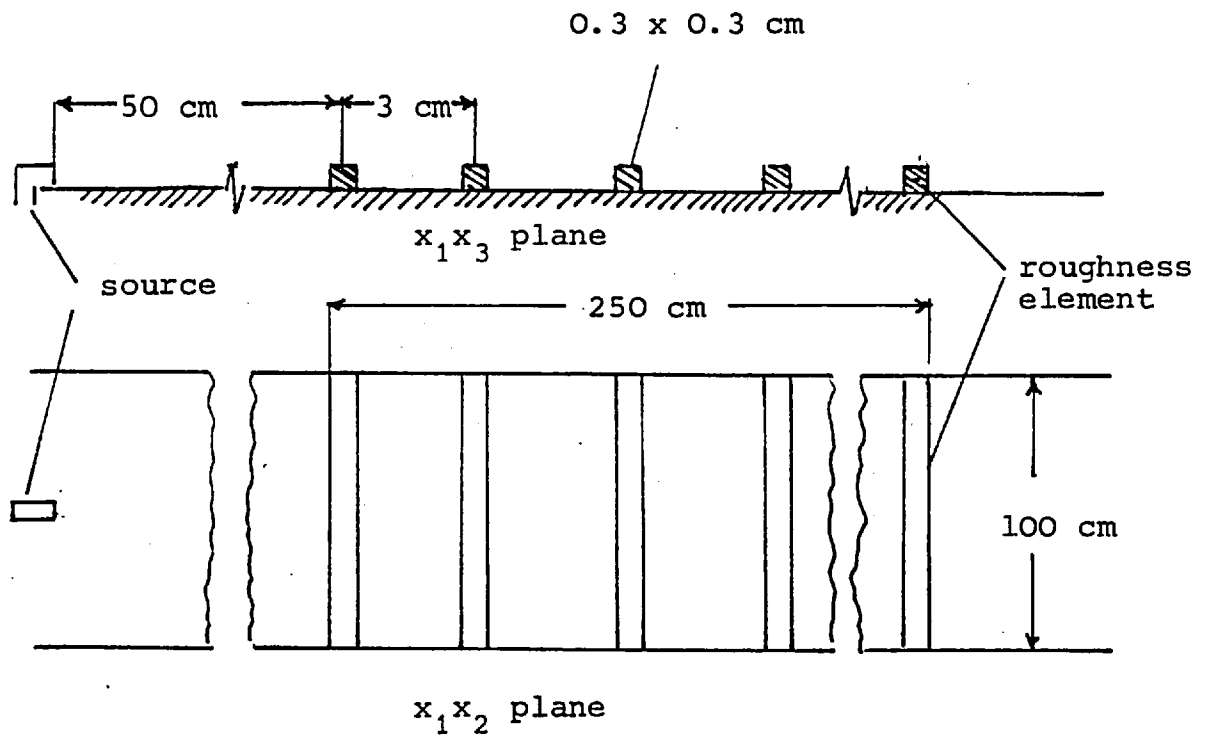


Figure 5.4 Elevation and plan views of positioning of roughness elements

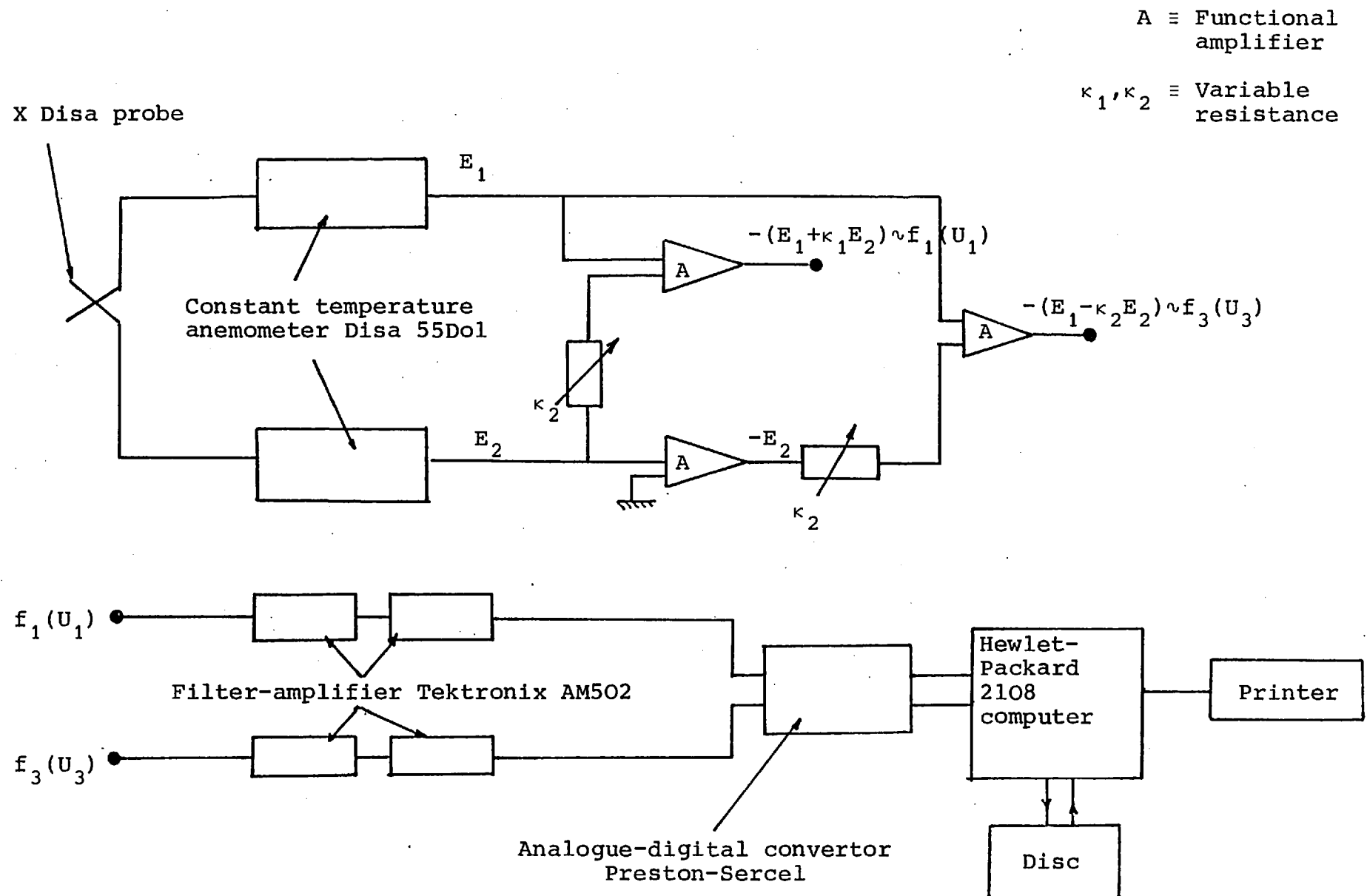


Figure 5.5 Hot wire circuitry

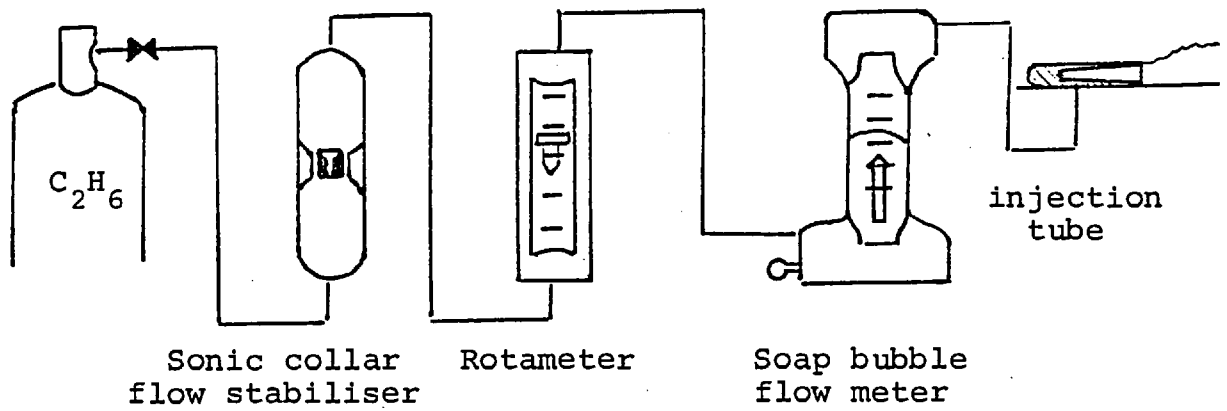


Figure 5.6 Arrangement for introduction and measurement of tracer stream

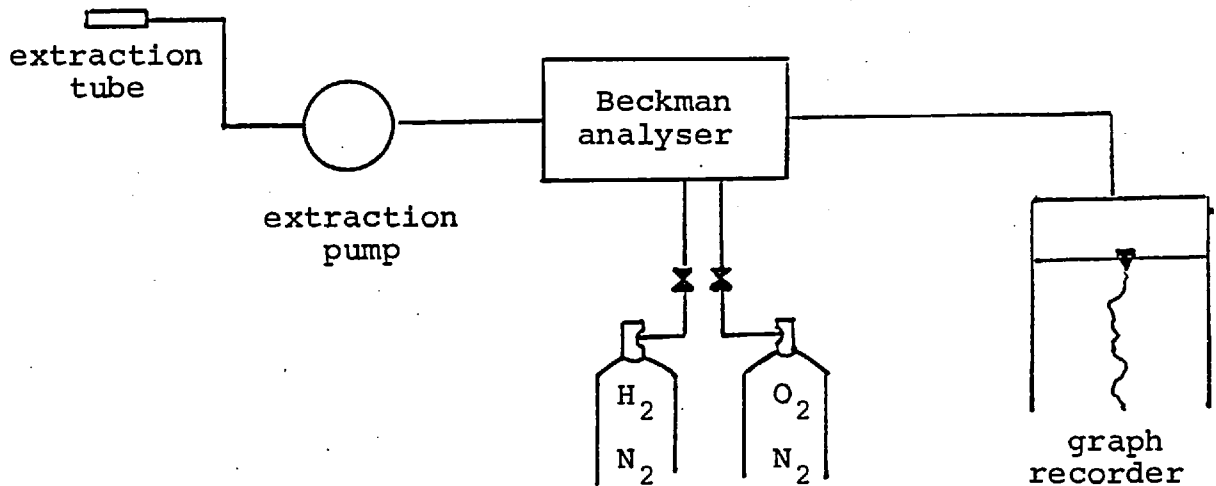


Figure 5.7 Sample extracting and concentration measuring apparatus

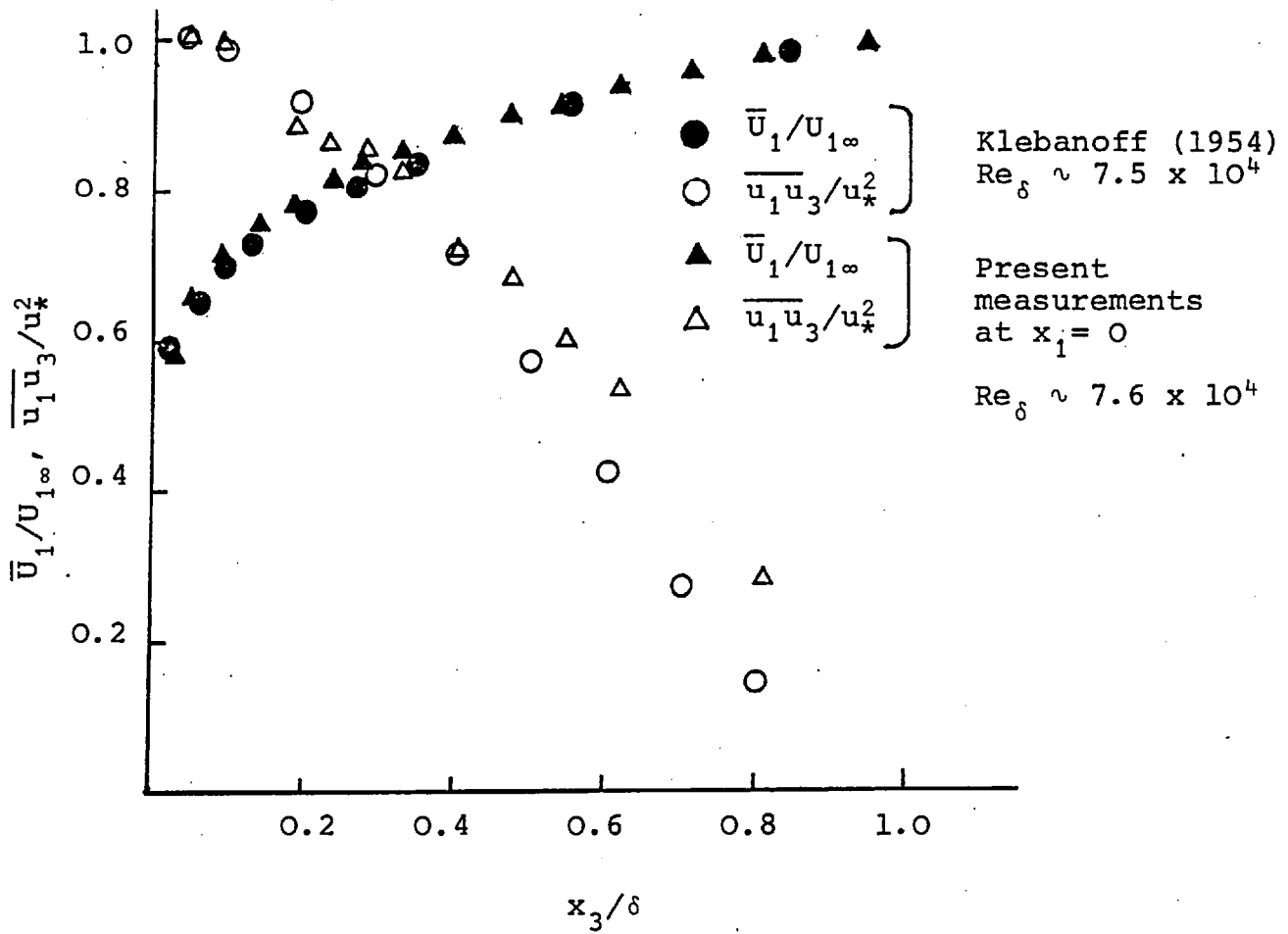


Figure 5.8 Measured distribution of mean streamwise velocity and turbulent shear stress in a turbulent boundary layer.

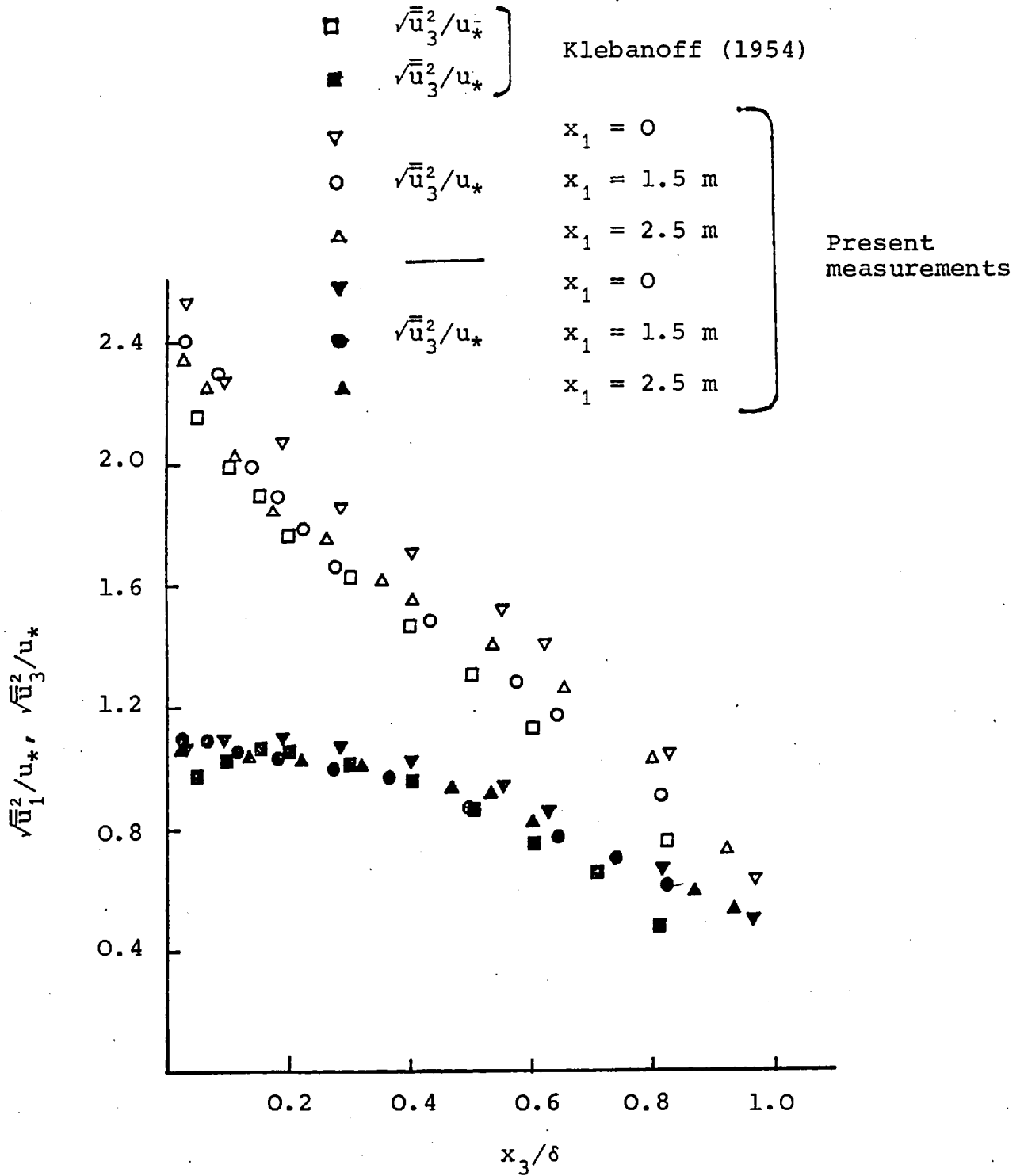


Figure 5.9 Measured distribution of the normal stresses at various downstream locations in boundary layer flow

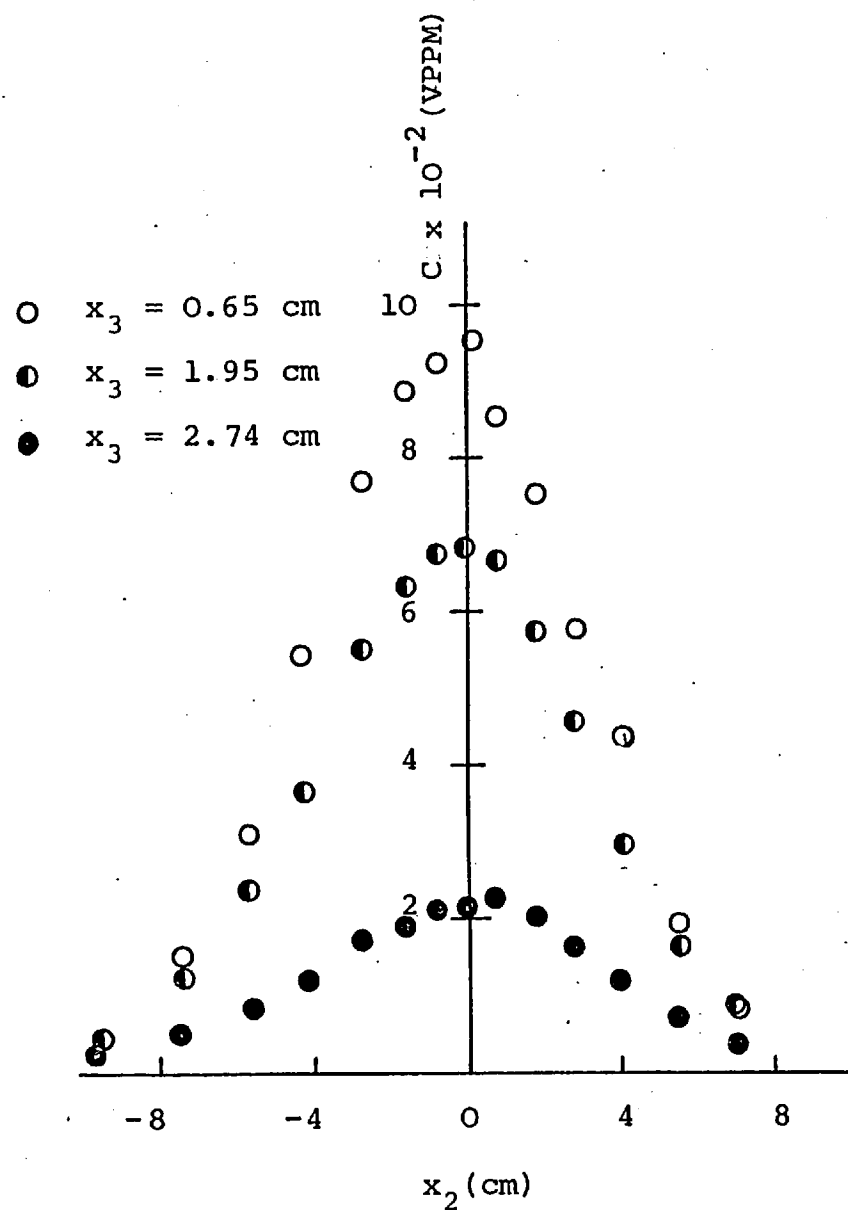


Figure 5.10 Measured lateral concentration profiles at various heights at $x_1 = 1$ m for a ground release and a continuously smooth surface

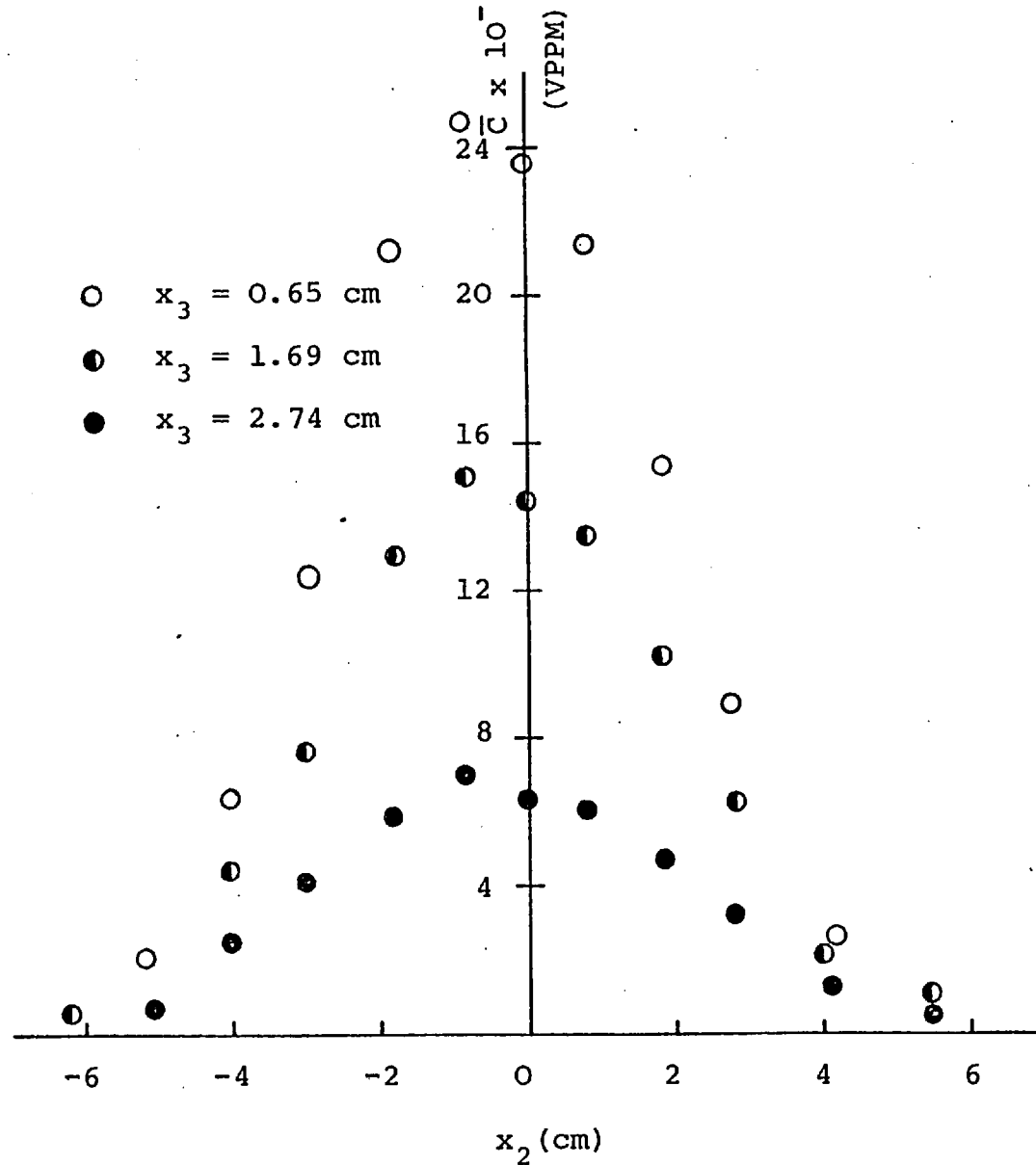


Figure 5.11 Measured concentration profiles at various heights at $x_1 = 0.5$ m for a ground release and a continuously smooth surface

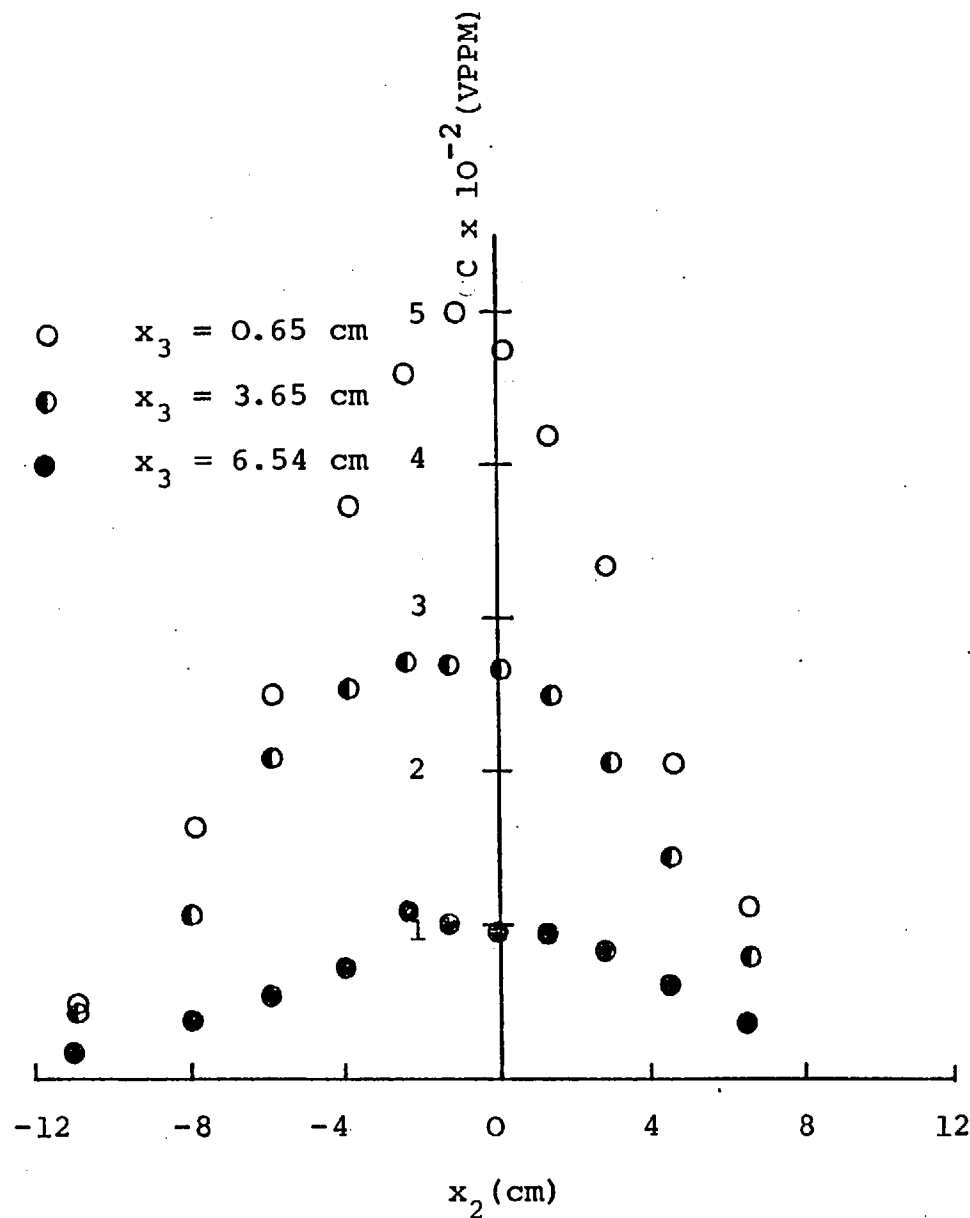


Figure 5.12 Measured lateral concentration profiles at $x_1 = 1.5$ m for a ground release and a continuously smooth surface

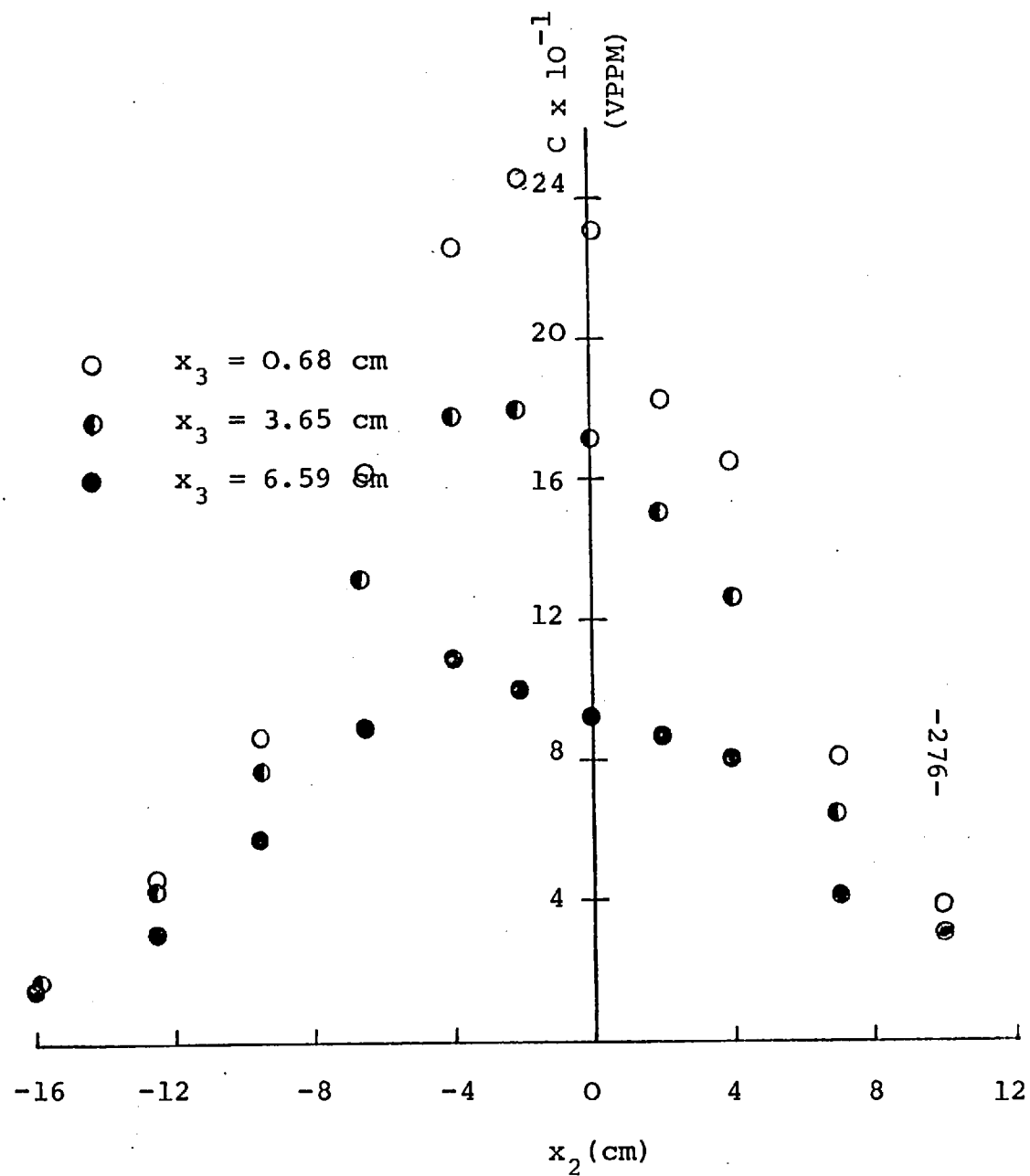


Figure 5.13 Measured lateral concentration profiles at various heights at $x_1 = 2.5$ m for a ground release and a continuously smooth surface

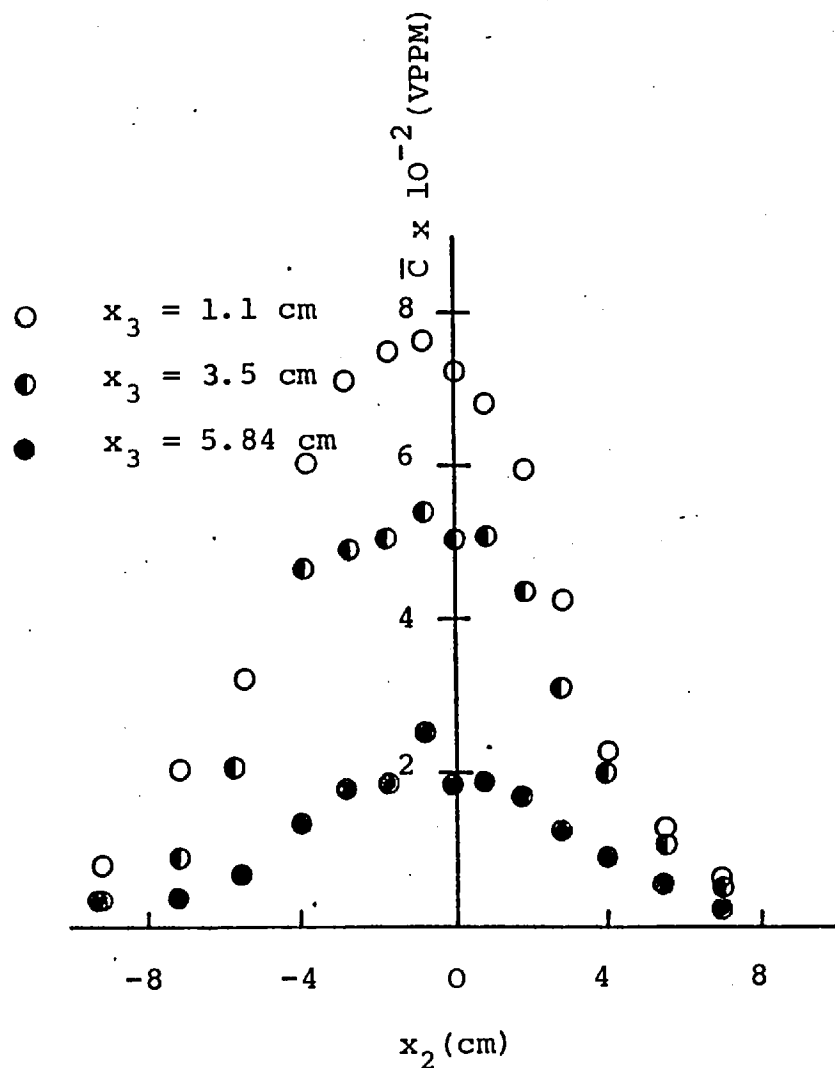


Figure 5.14 Measured lateral concentration profiles at various heights and a partially rough surface

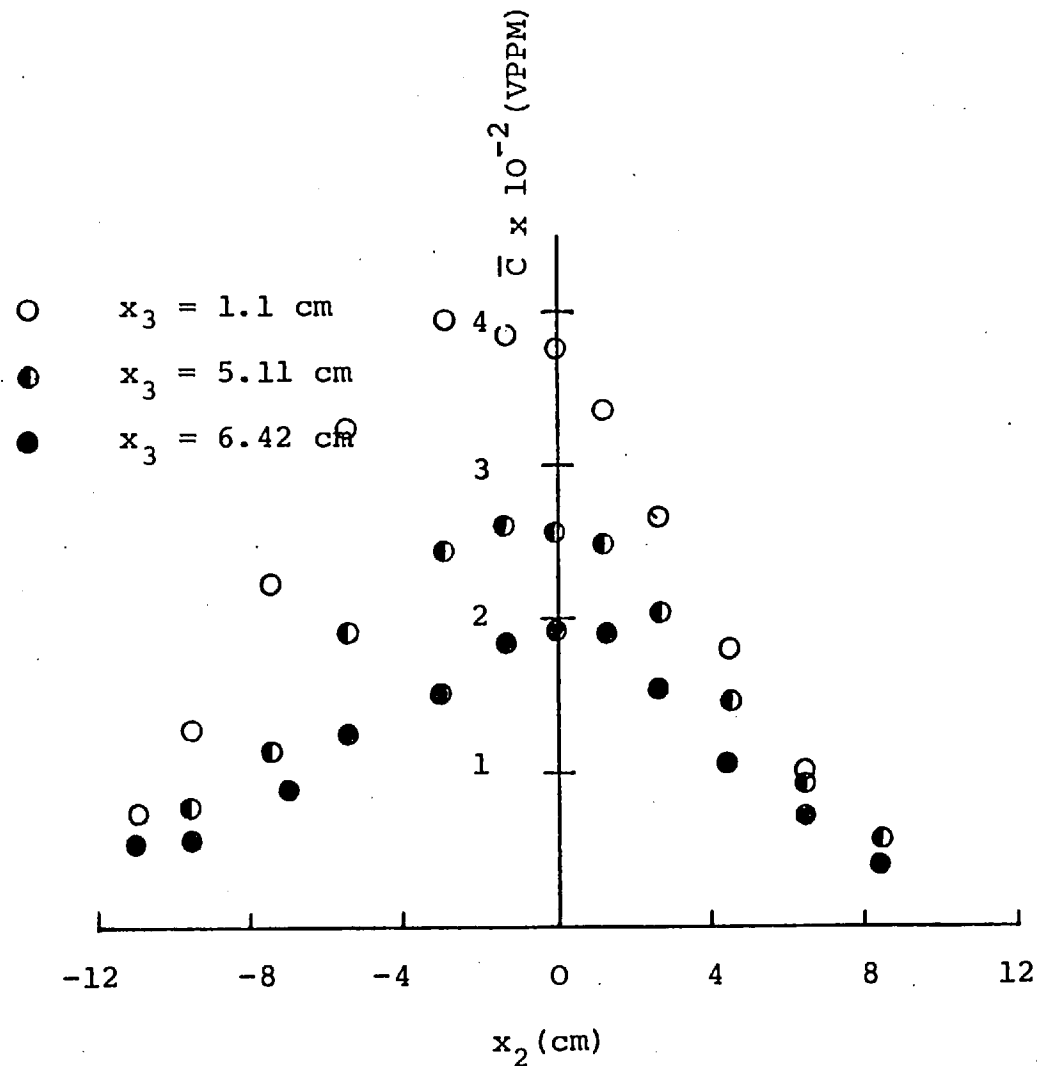


Figure 5.15 Measured lateral concentration profiles at various heights at $x_1 = 1.5$ m for a ground release and a partially rough surface

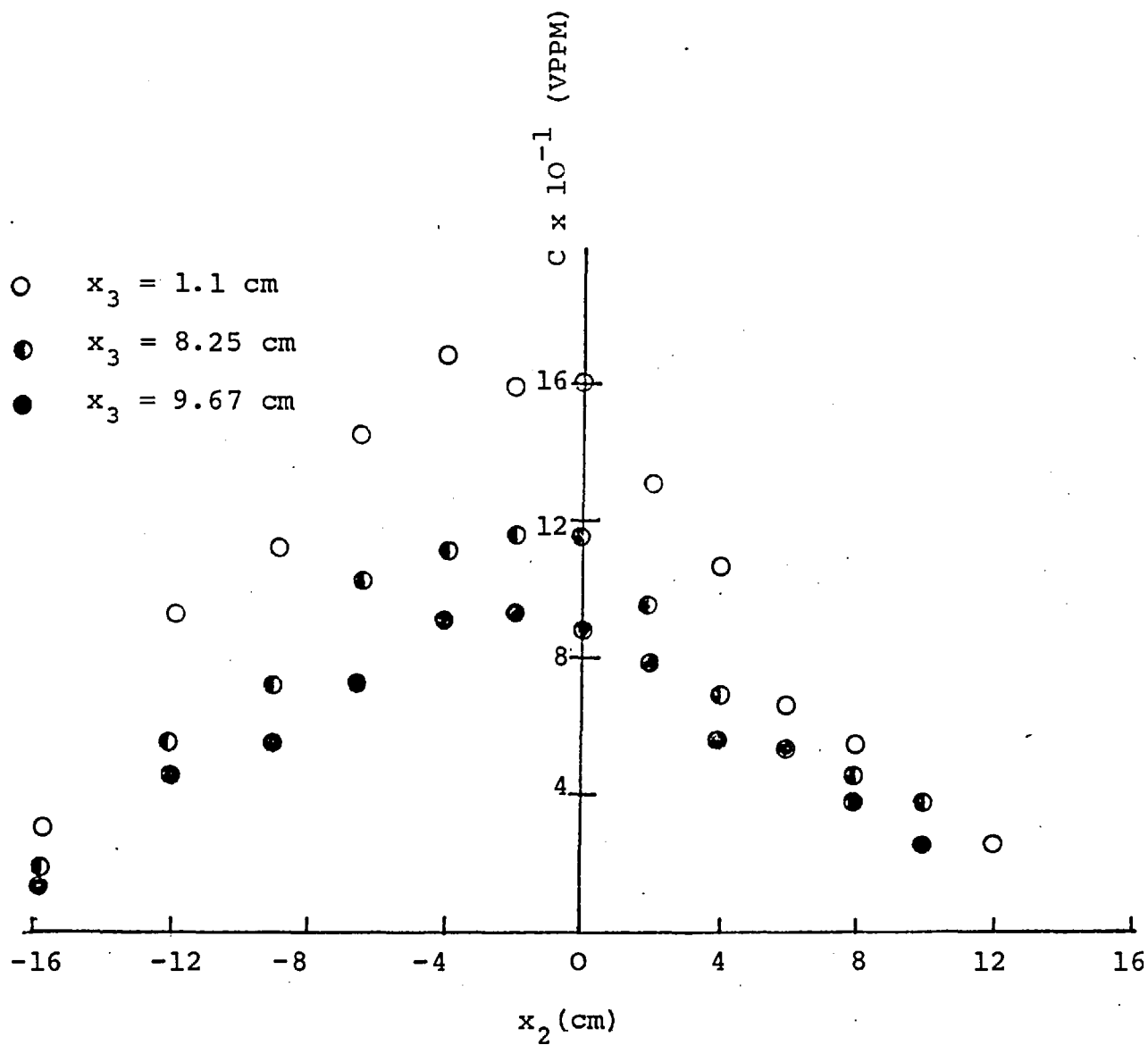


Figure 5.16 Measured lateral concentration profile at various heights at $x_1 = 2.5 \text{ m}$ for a ground release and a partially rough surface

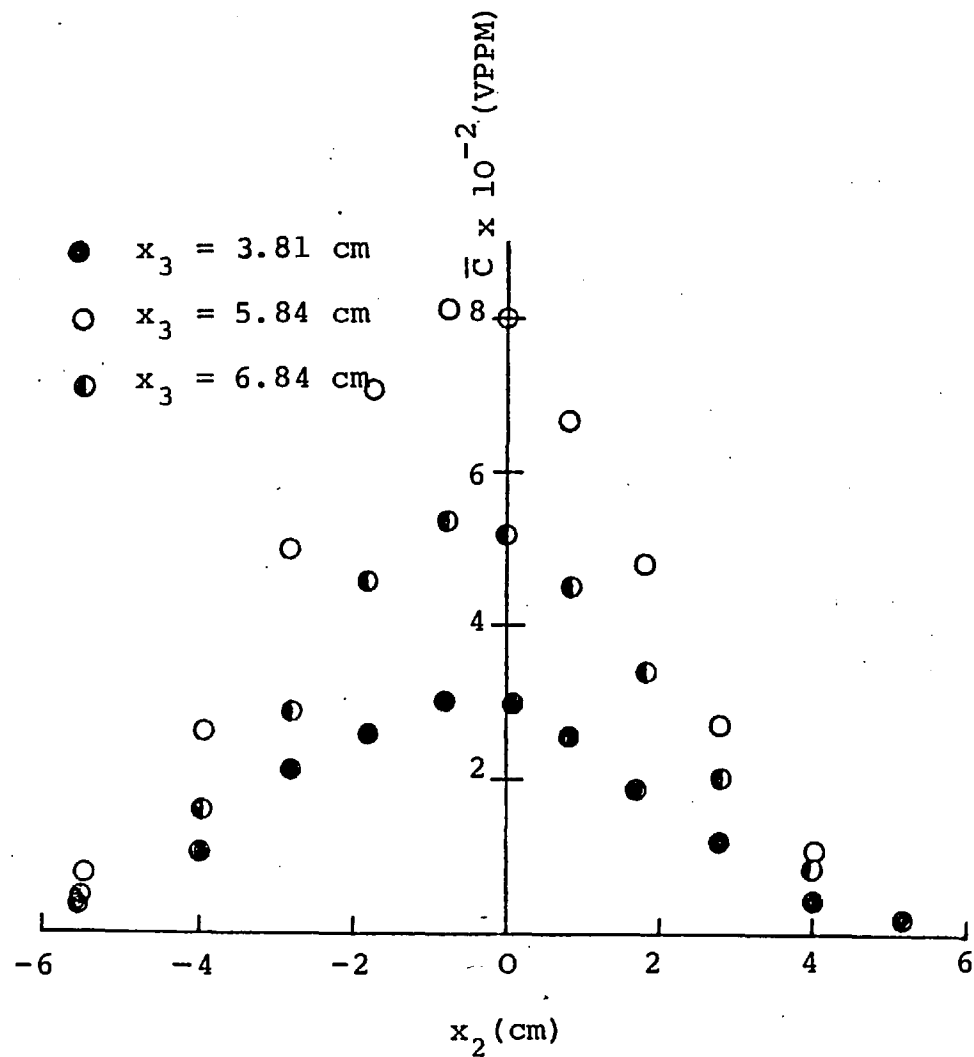


Figure 5.17 Measured lateral concentration profiles at various heights at $x_1 = 0.5$ m for an elevated source

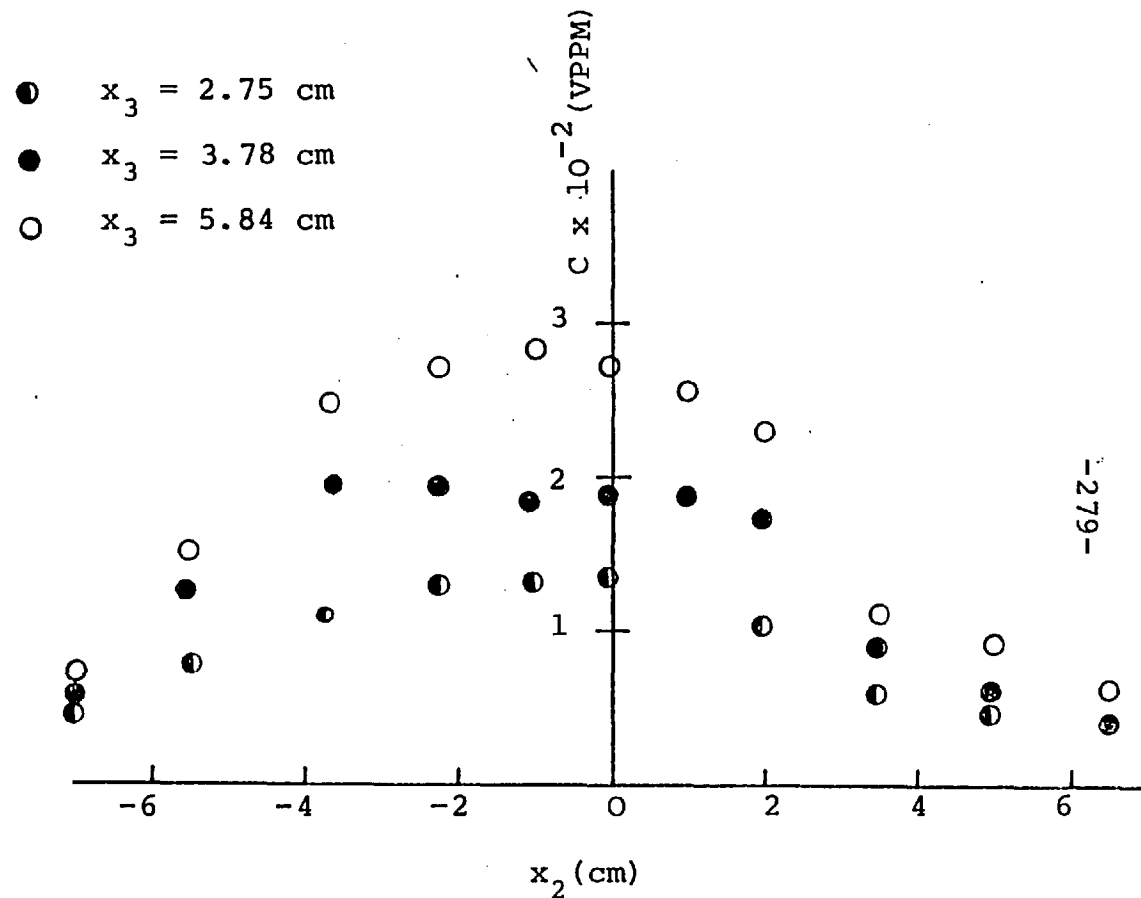


Figure 5.18 Measured lateral concentration profiles at various heights at $x_1 = 1$ m for an elevated source

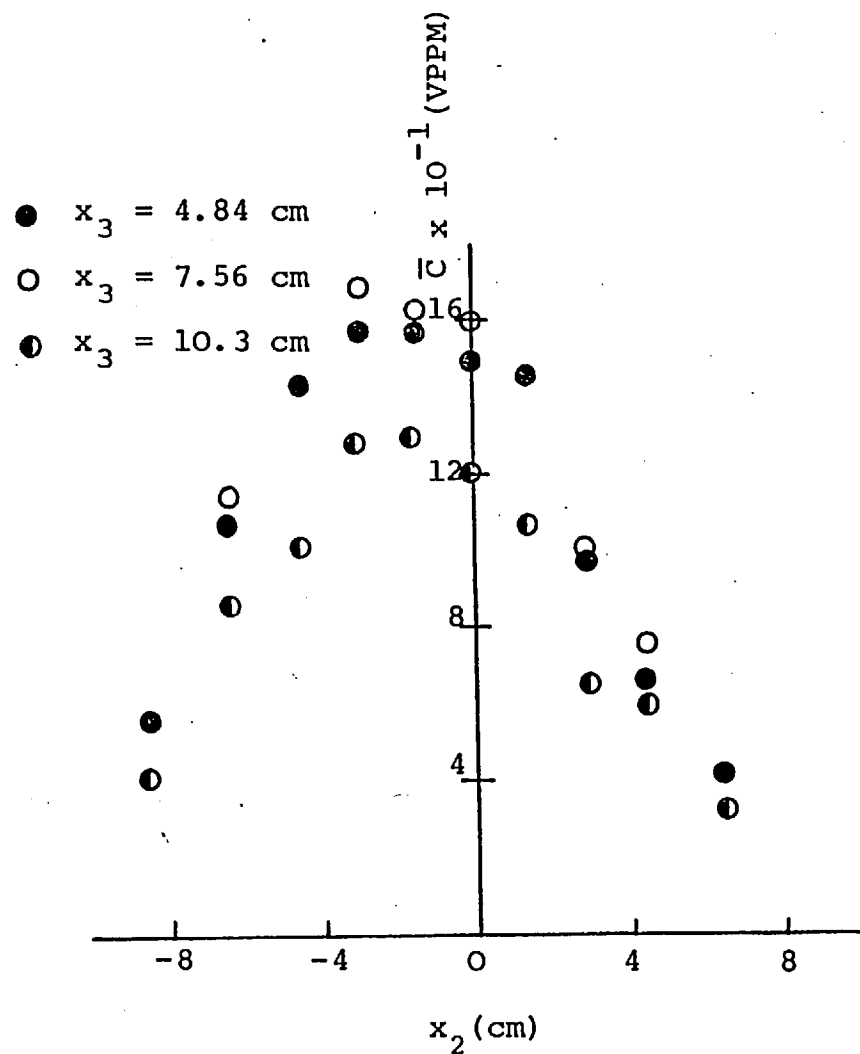


Figure 5.19 Measured lateral concentration profiles at various lengths at $x_1 = 1.5$ m for an elevated source

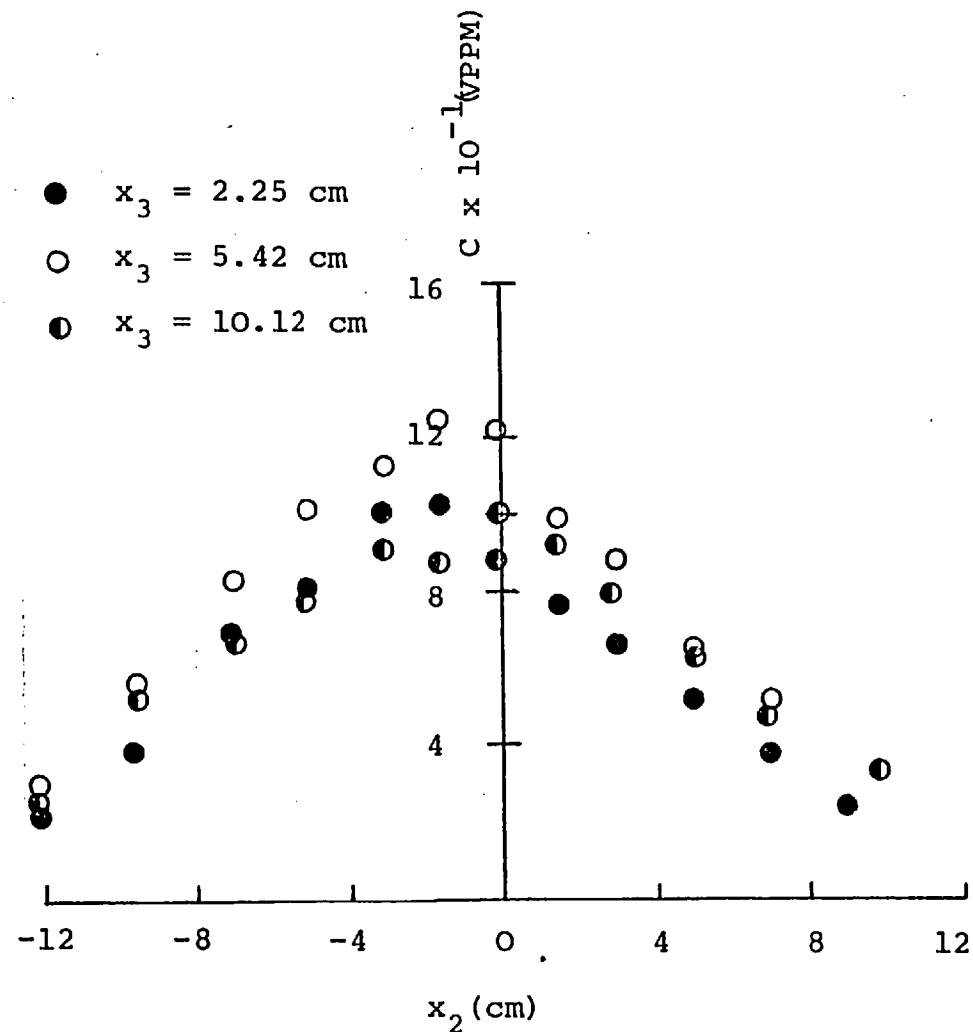


Figure 5.20 Measured lateral concentration profiles at various heights at $x_1 = 2$ m for an elevated release

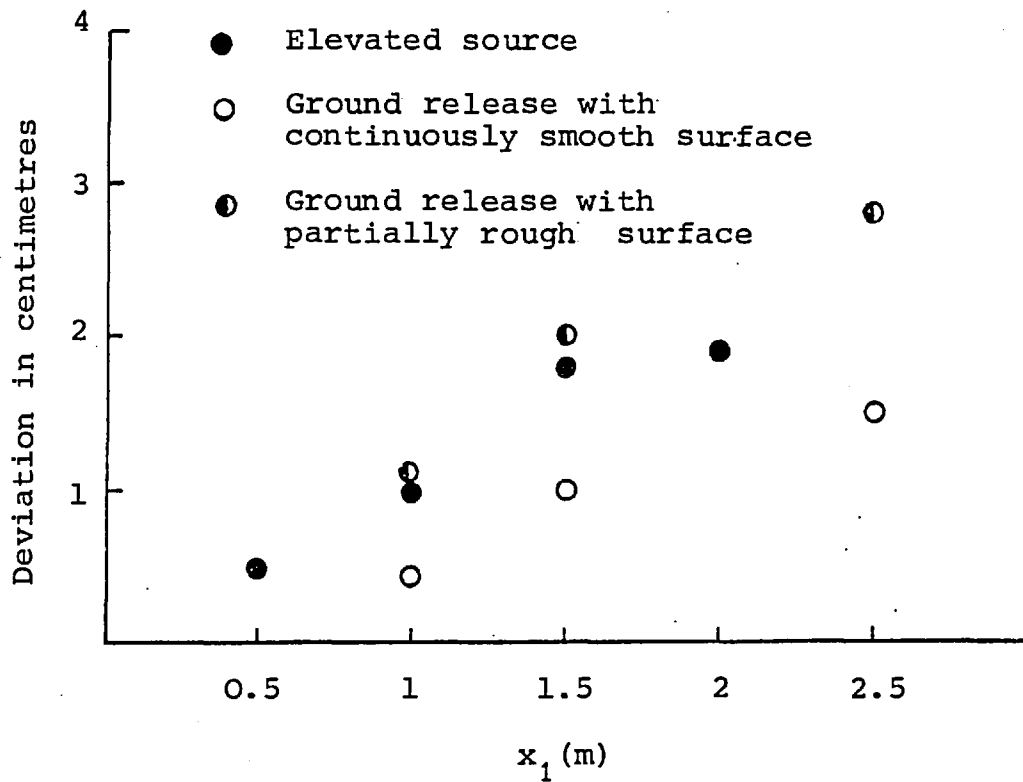


Figure 5.21 Lateral deviation of the centre line of the plume from the wind tunnel's symmetry axis

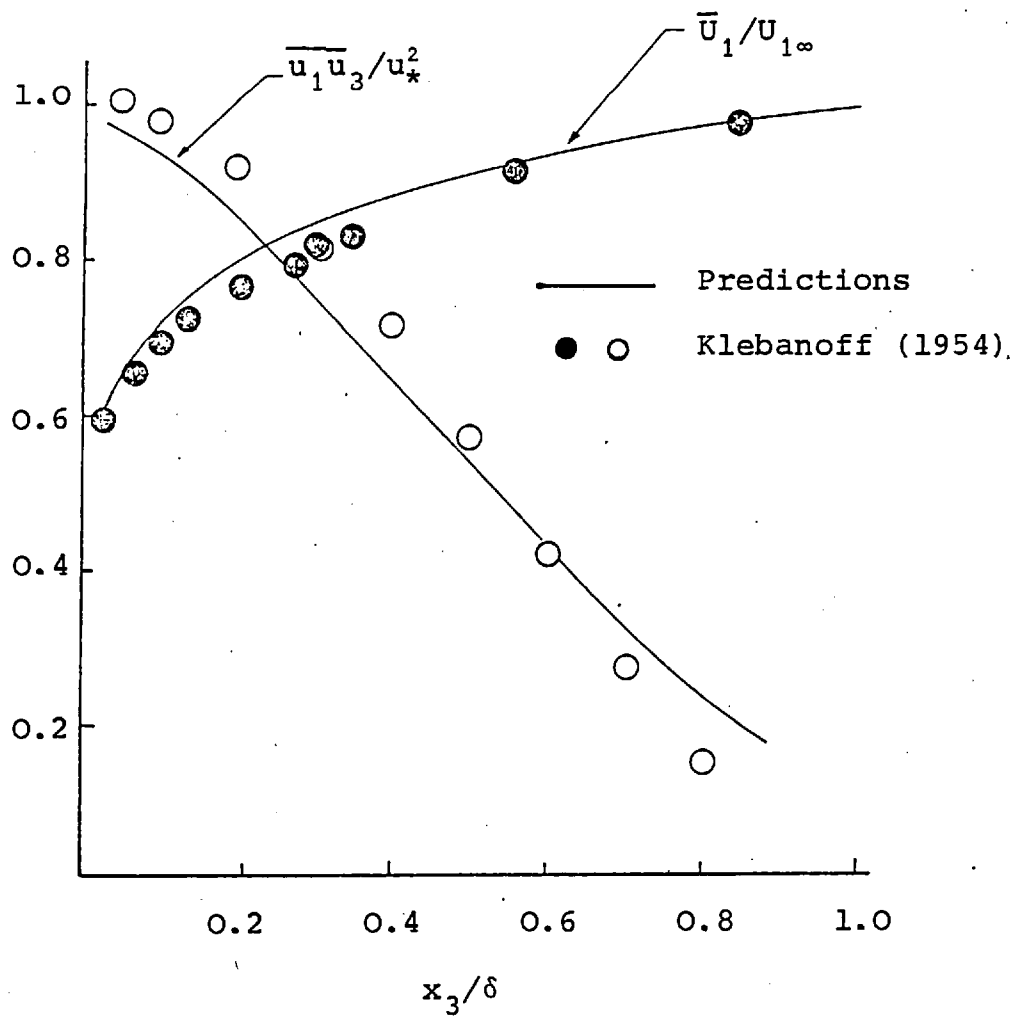


Figure 6.1 Comparison of measured and predicted mean velocity and shear stress profiles across a boundary layer

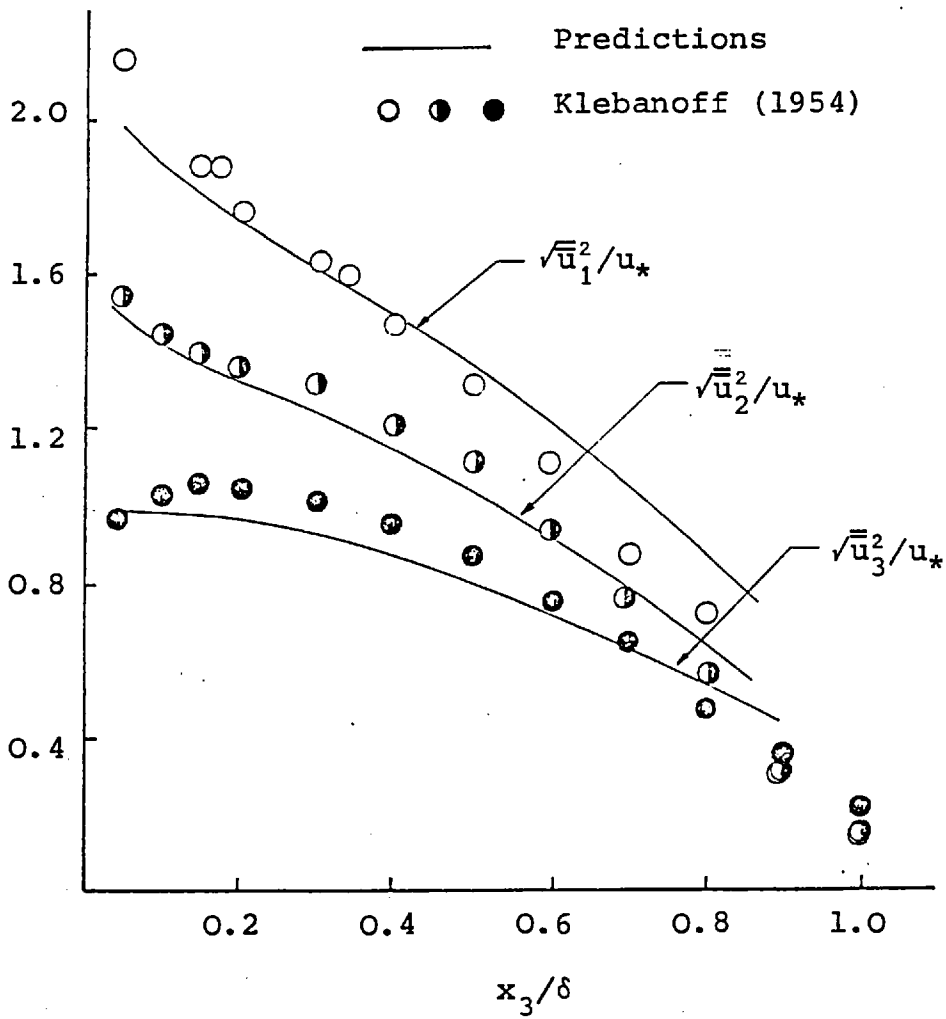


Figure 6.2 Comparison between predicted and measured turbulence intensity profiles across a flat plate boundary layer

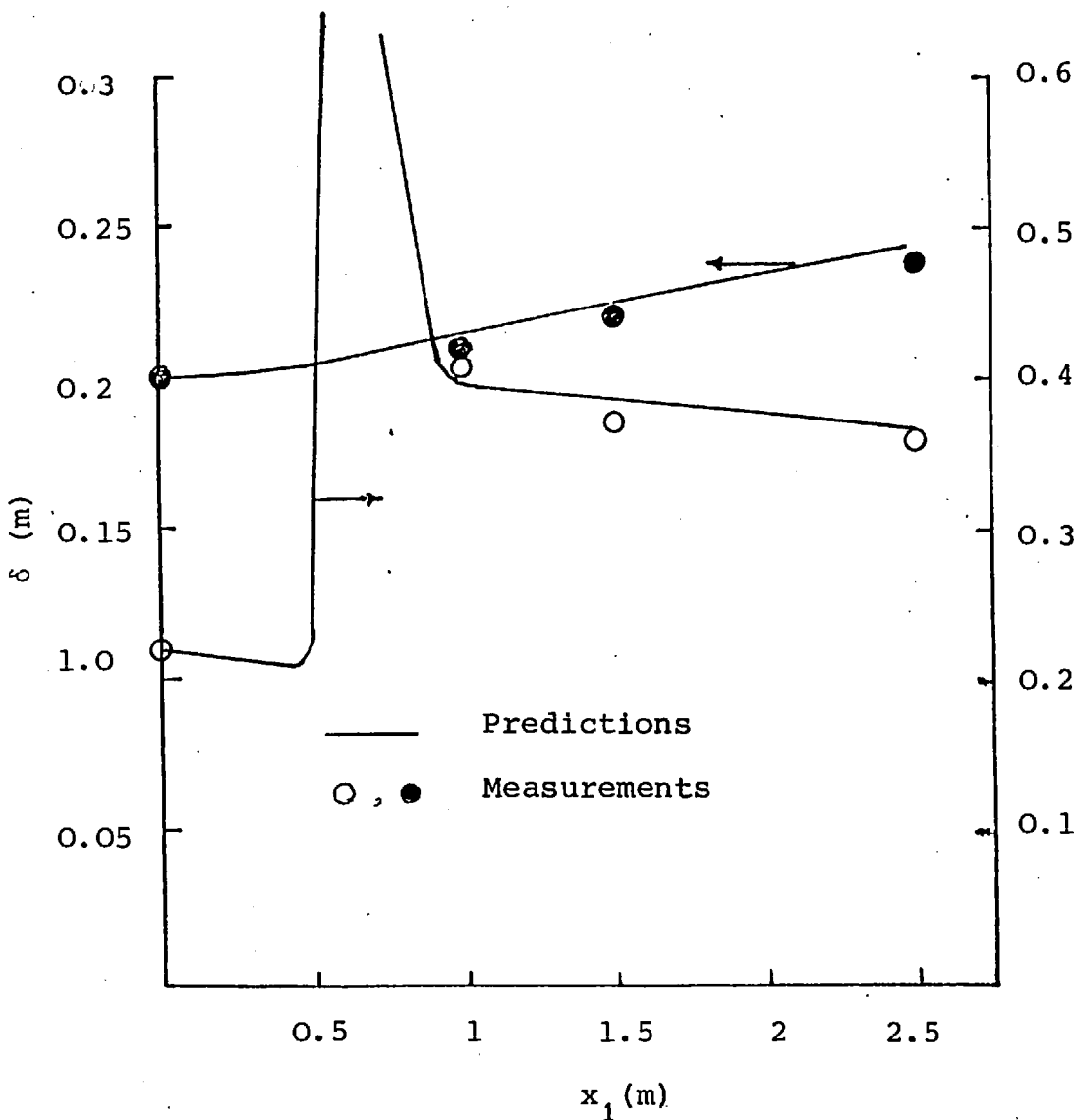


Figure 6.3 Variation of shear velocity and boundary layer thickness with downstream distance for boundary layer flow over a partially rough surface

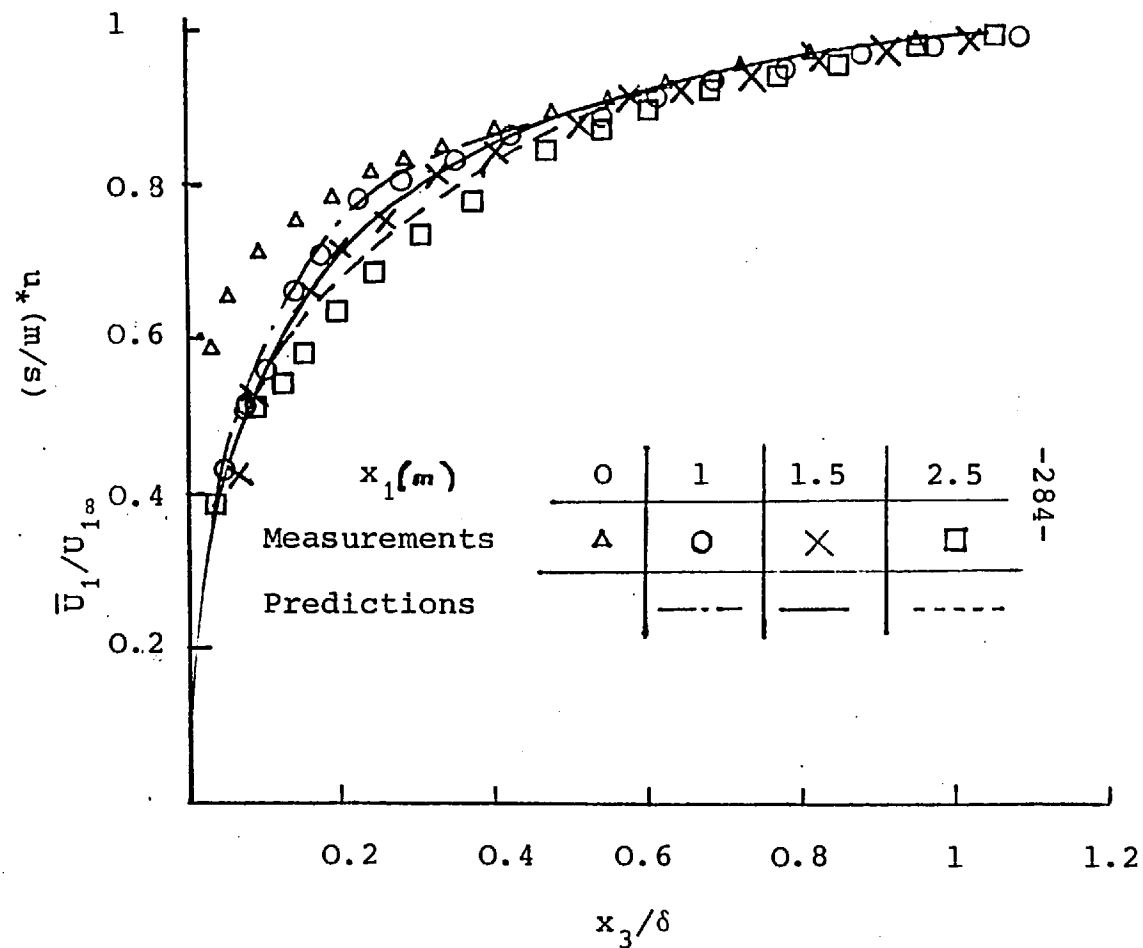


Figure 6.4 Development of mean streamwise velocity profile with downstream distance for a boundary layer flow over a partially rough surface

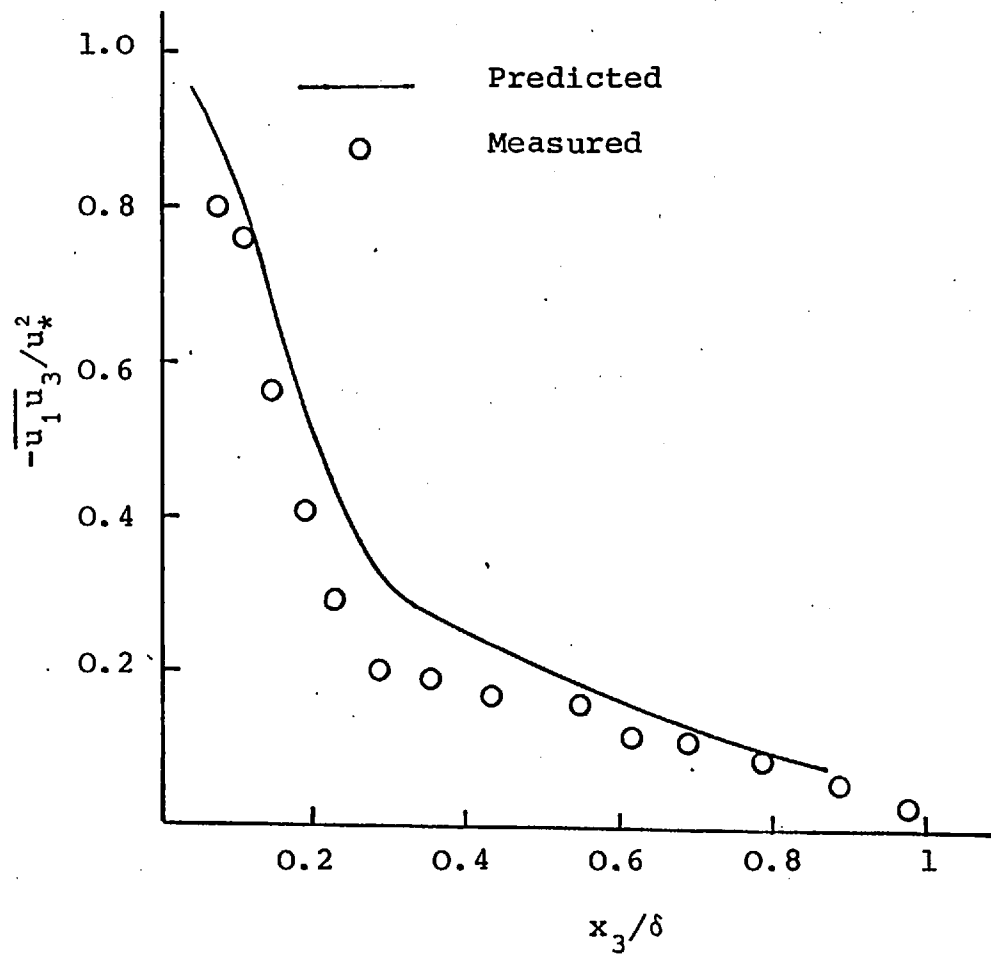


Figure 6.5 Normalised shear stress profile at $x_1 = 1$ m for a flow over a partially rough surface

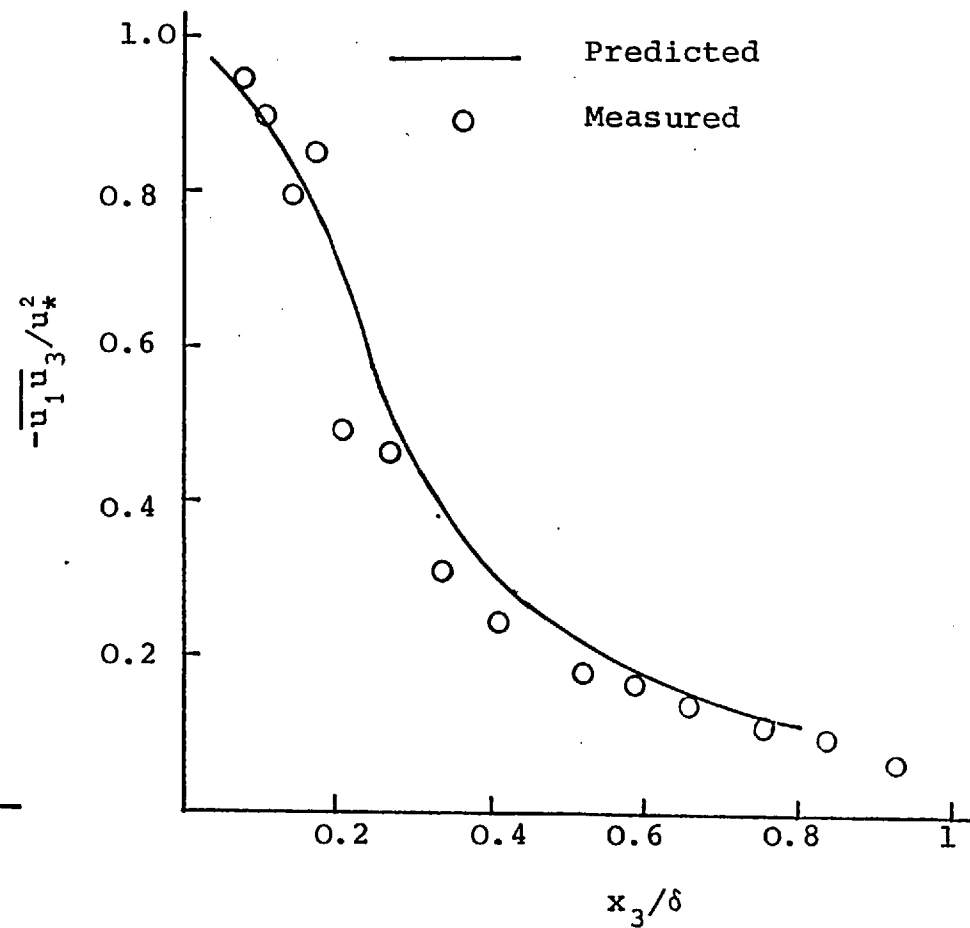


Figure 6.6 Normalised shear stress profile at $x_1 = 1.5$ m for a flow over a partially rough surface

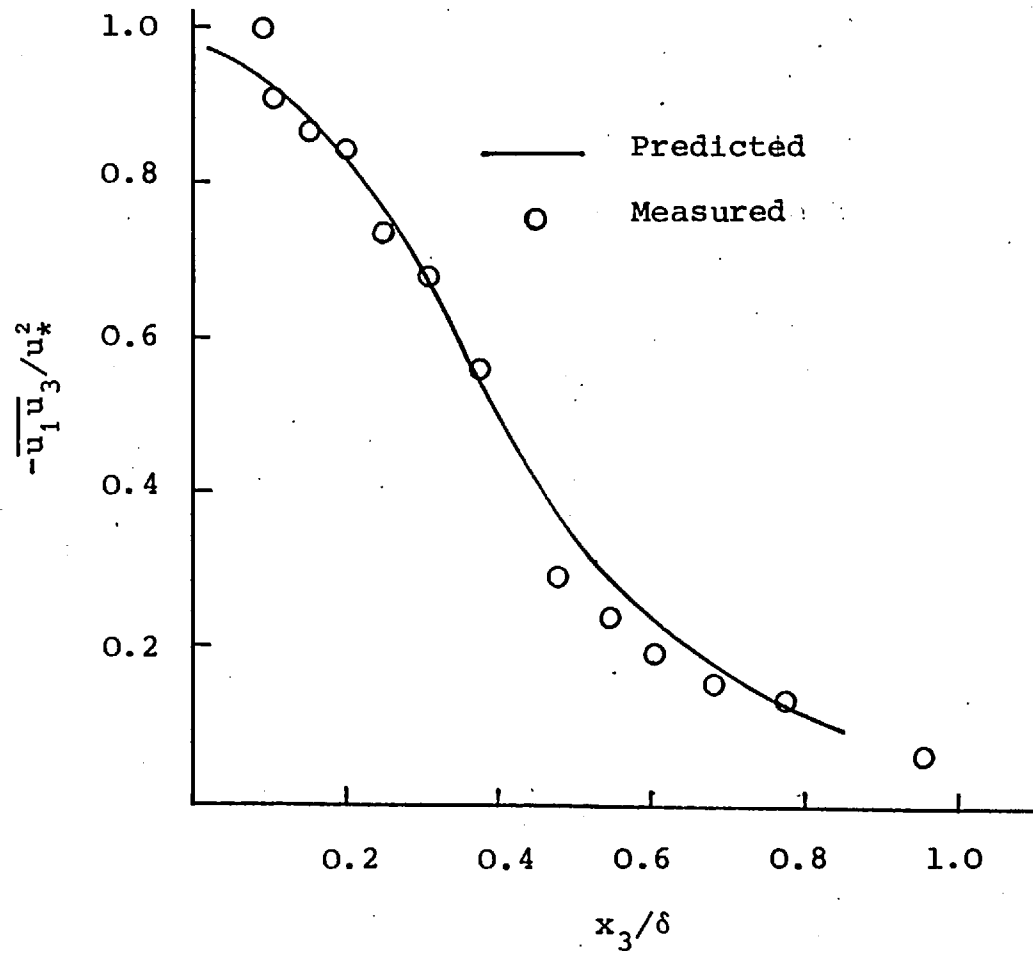


Figure 6.7 Normalised shear stress profile at $x_1 = 1$ m for a flow over a partially rough surface

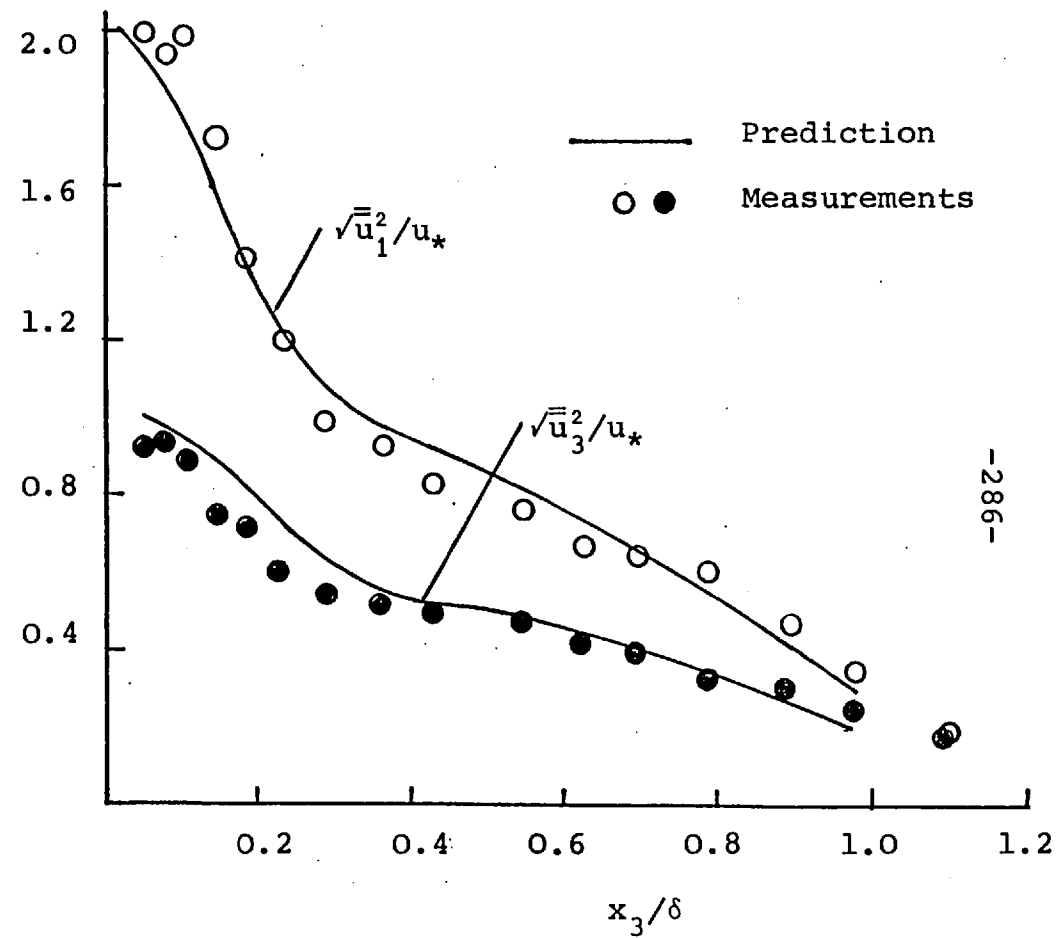


Figure 6.8 Normalised turbulence intensity profiles at $x_1 = 1$ m for a flow over a partially rough surface

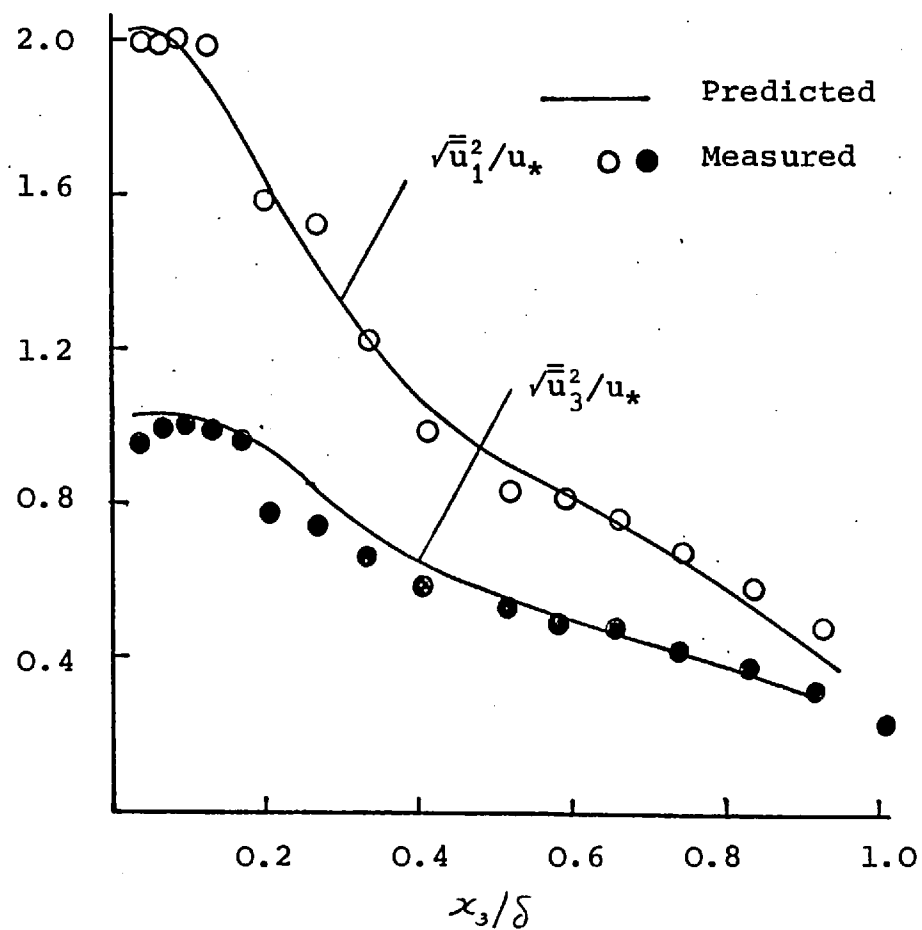


Figure 6.9 Normalised turbulence intensity profiles at $x_1 = 1.5$ for a flow over a partially rough surface

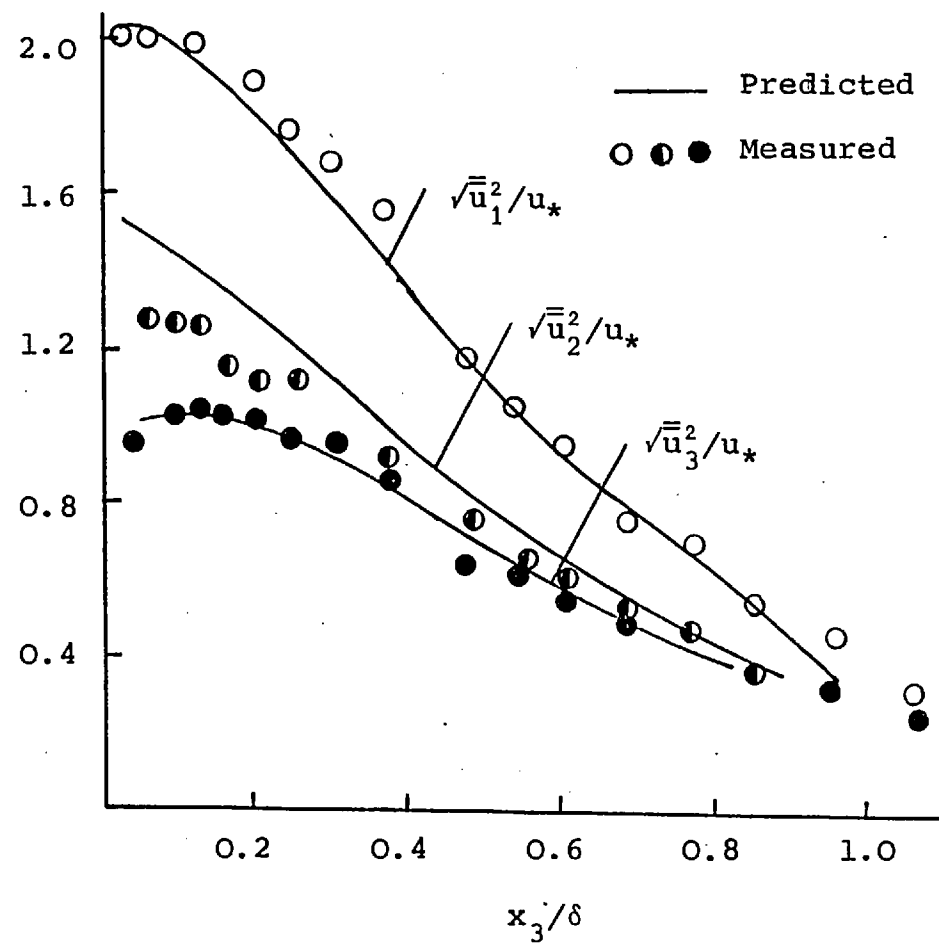


Figure 6.10 Normalised turbulence intensity profiles at $x_1 = 2.5$ for a flow over a partially rough surface

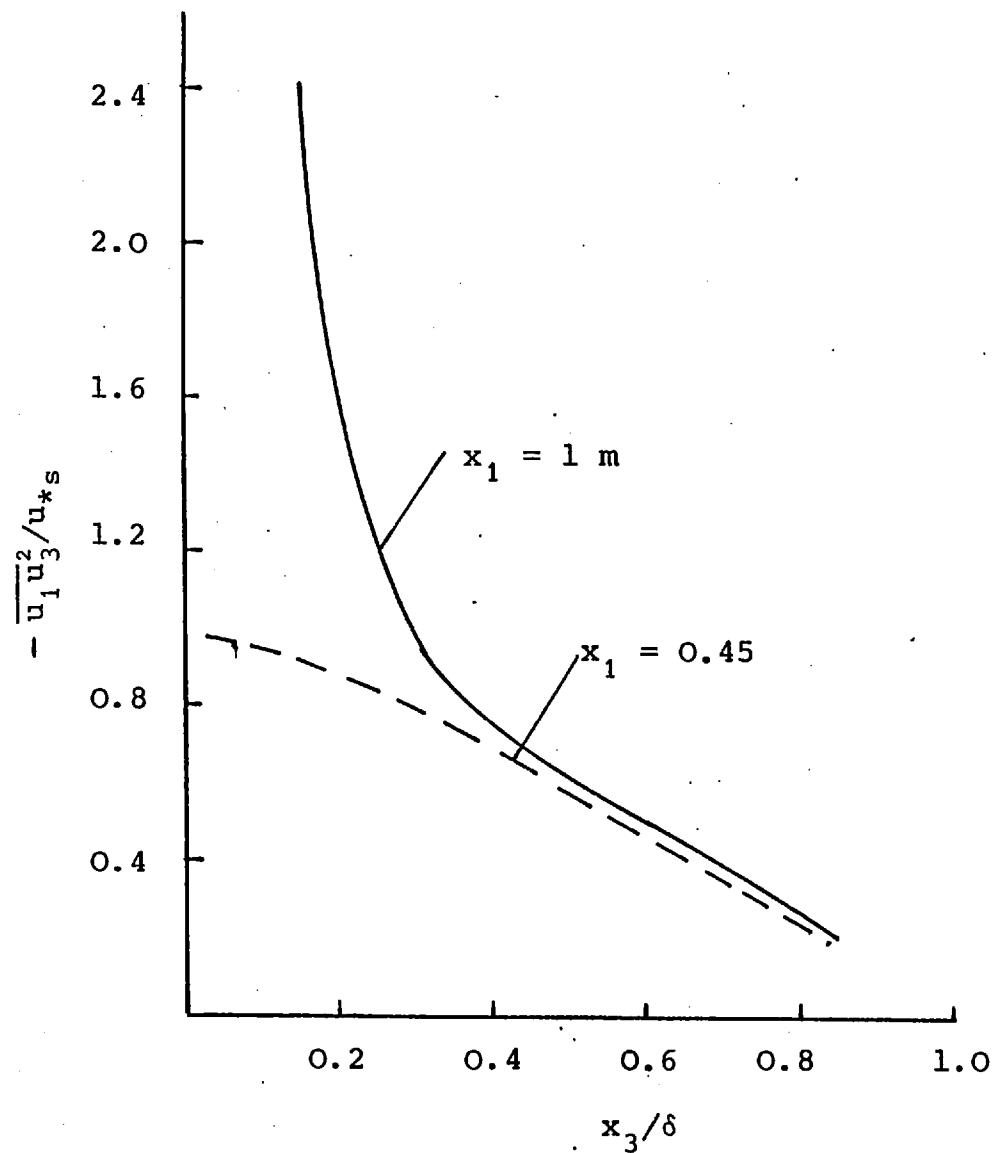


Figure 6.11 Shear stress profile at locations upstream and downstream of the change in roughness

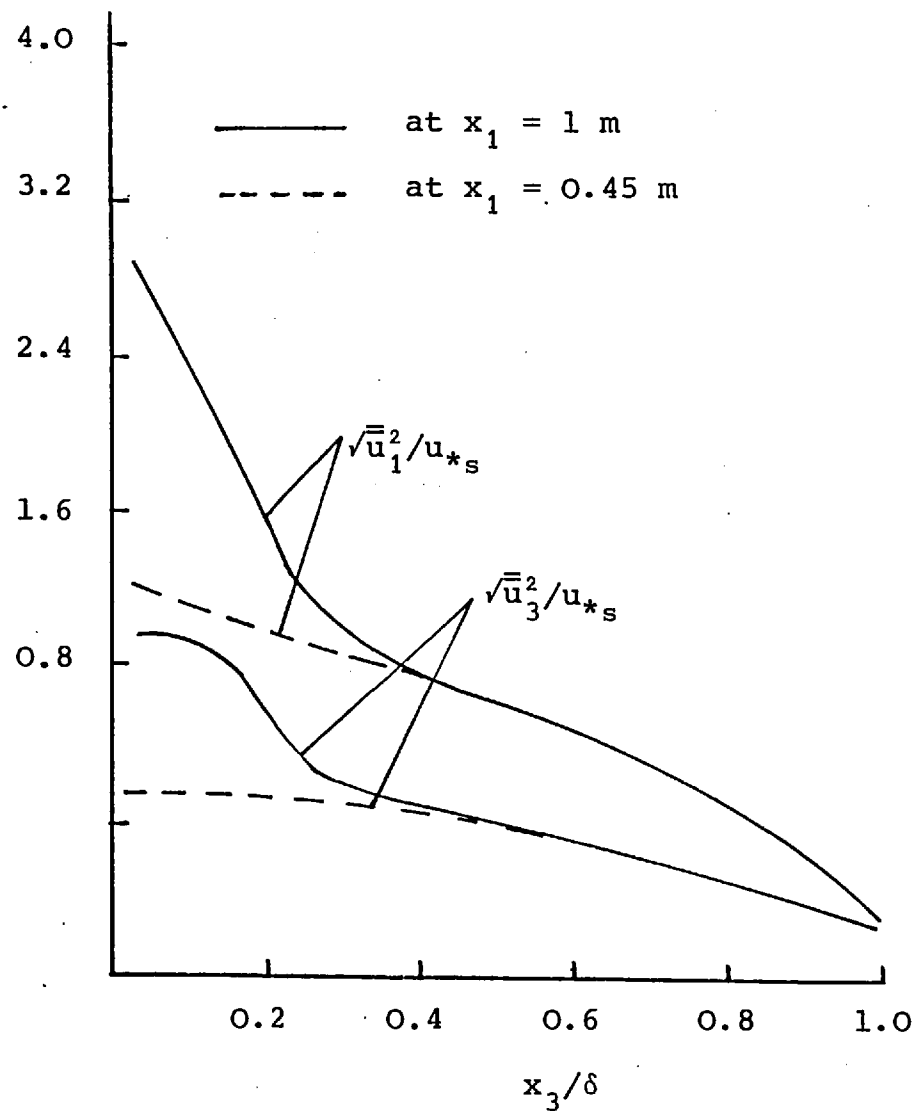


Figure 6.12 Turbulence intensity profiles at locations upstream and downstream of the change in roughness

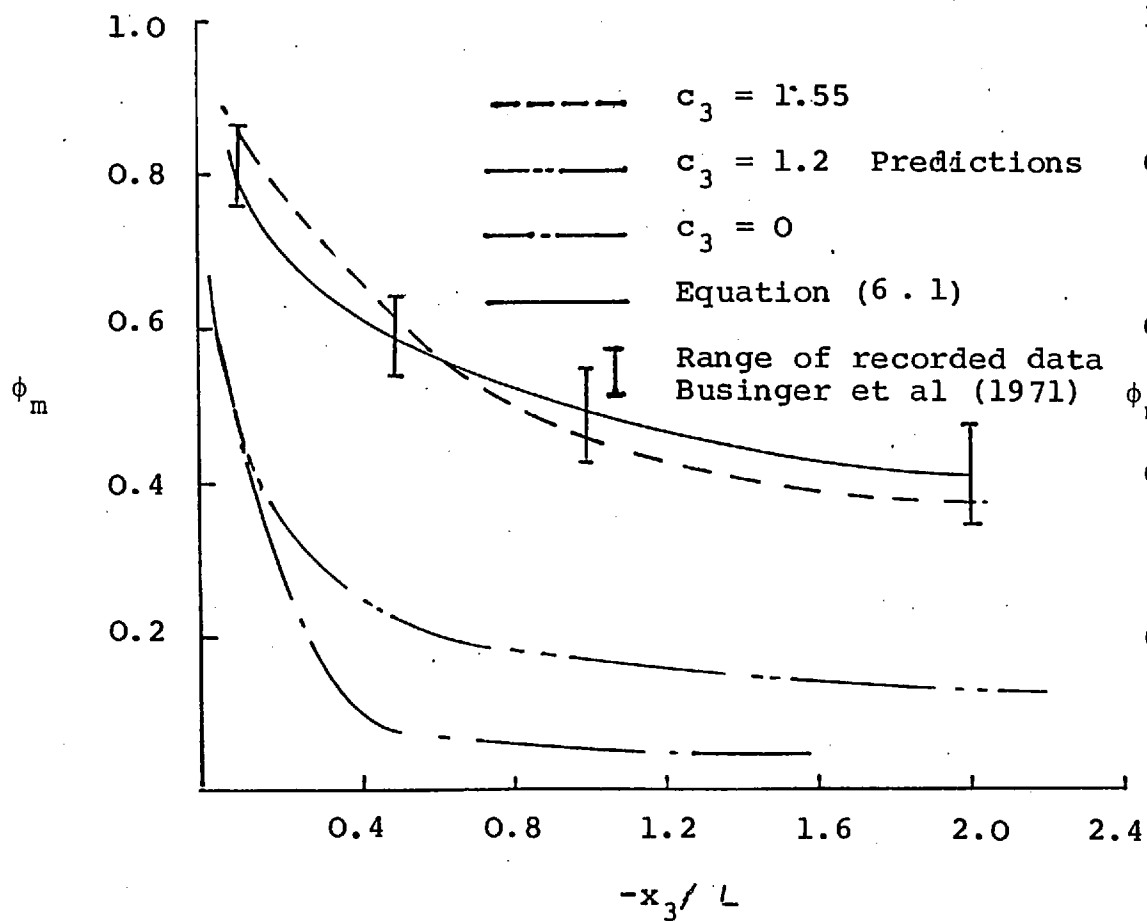


Figure 6.13 Effect of unstable stratification on normalised velocity gradient

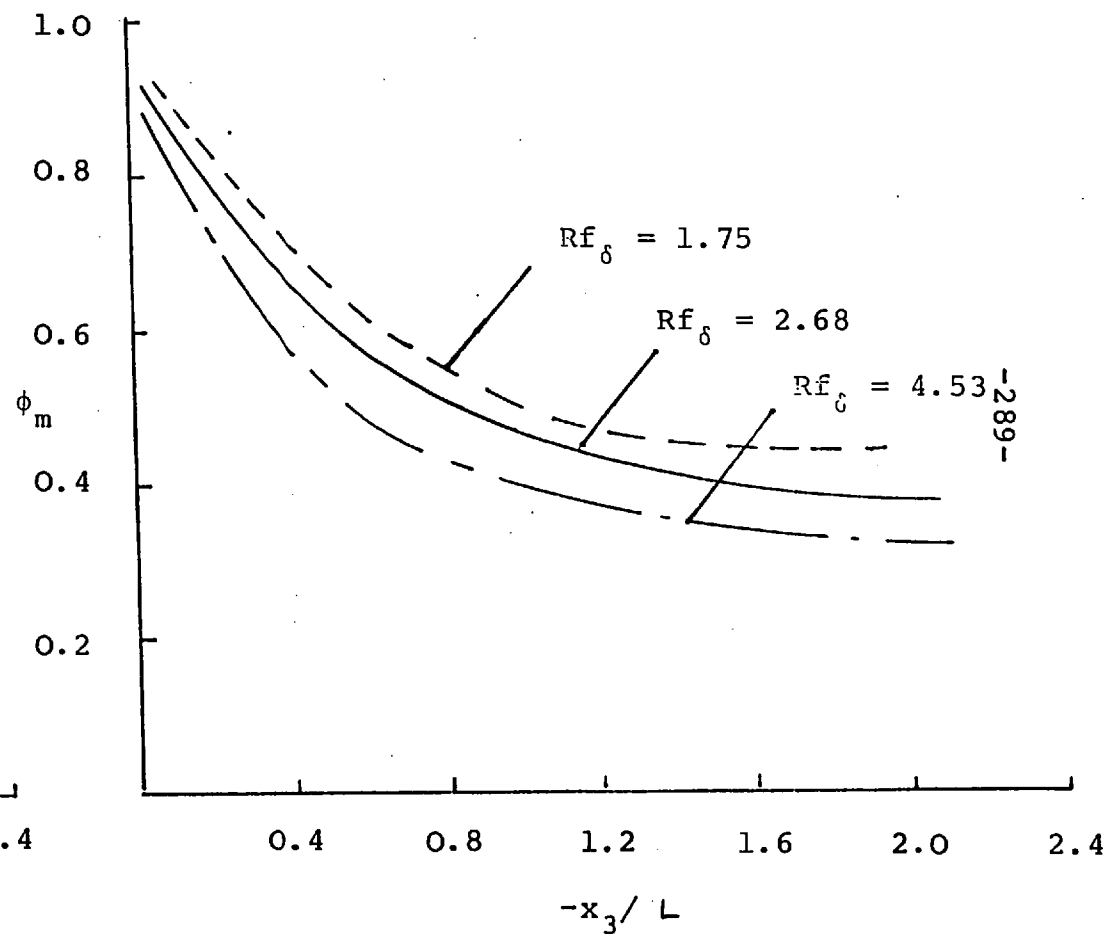


Figure 6.14 Predicted dependence of normalised velocity gradient on x_3/L and Rf_δ

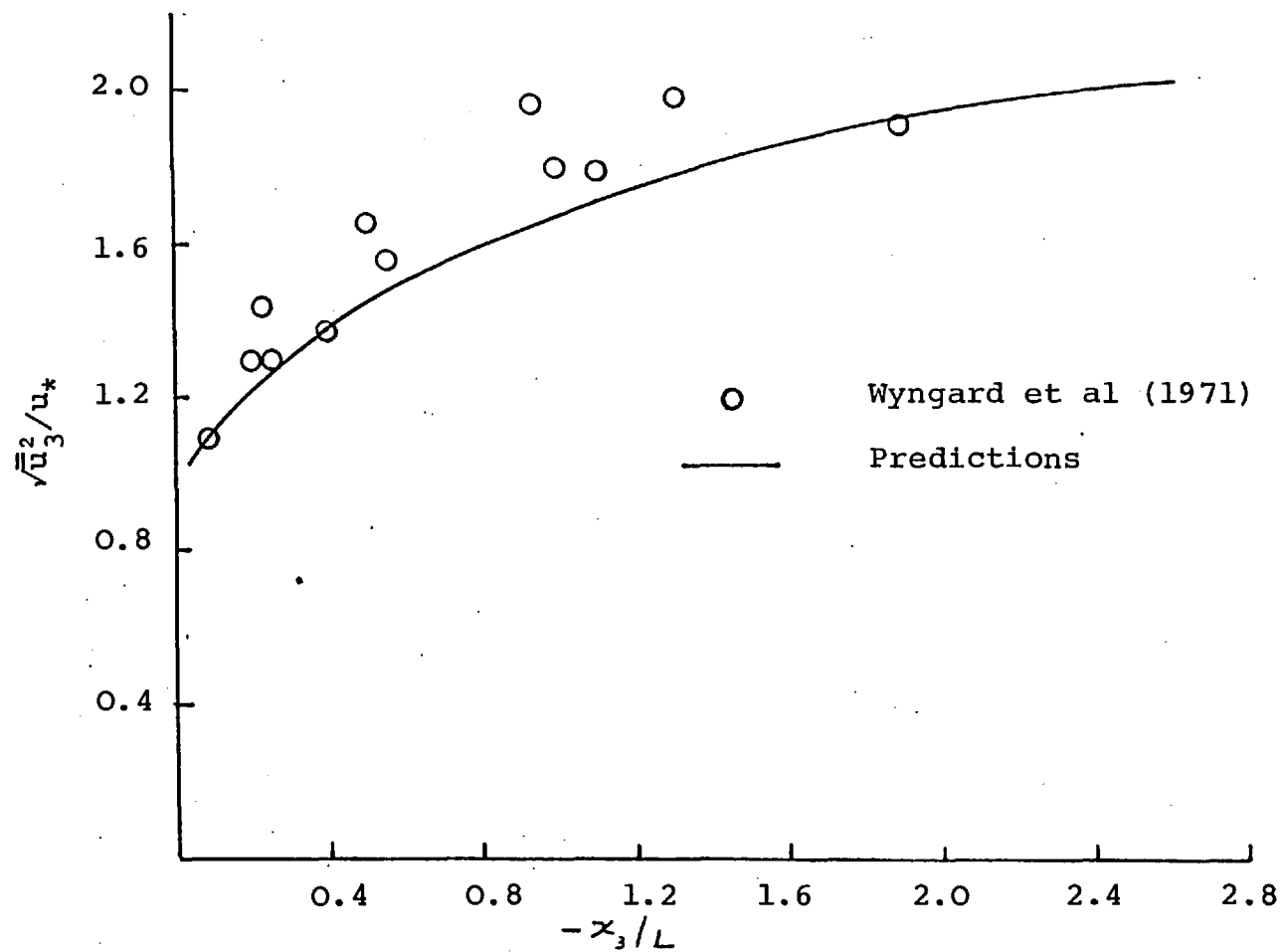


Figure 6.15 Dependence of vertical velocity fluctuation on x_3/L

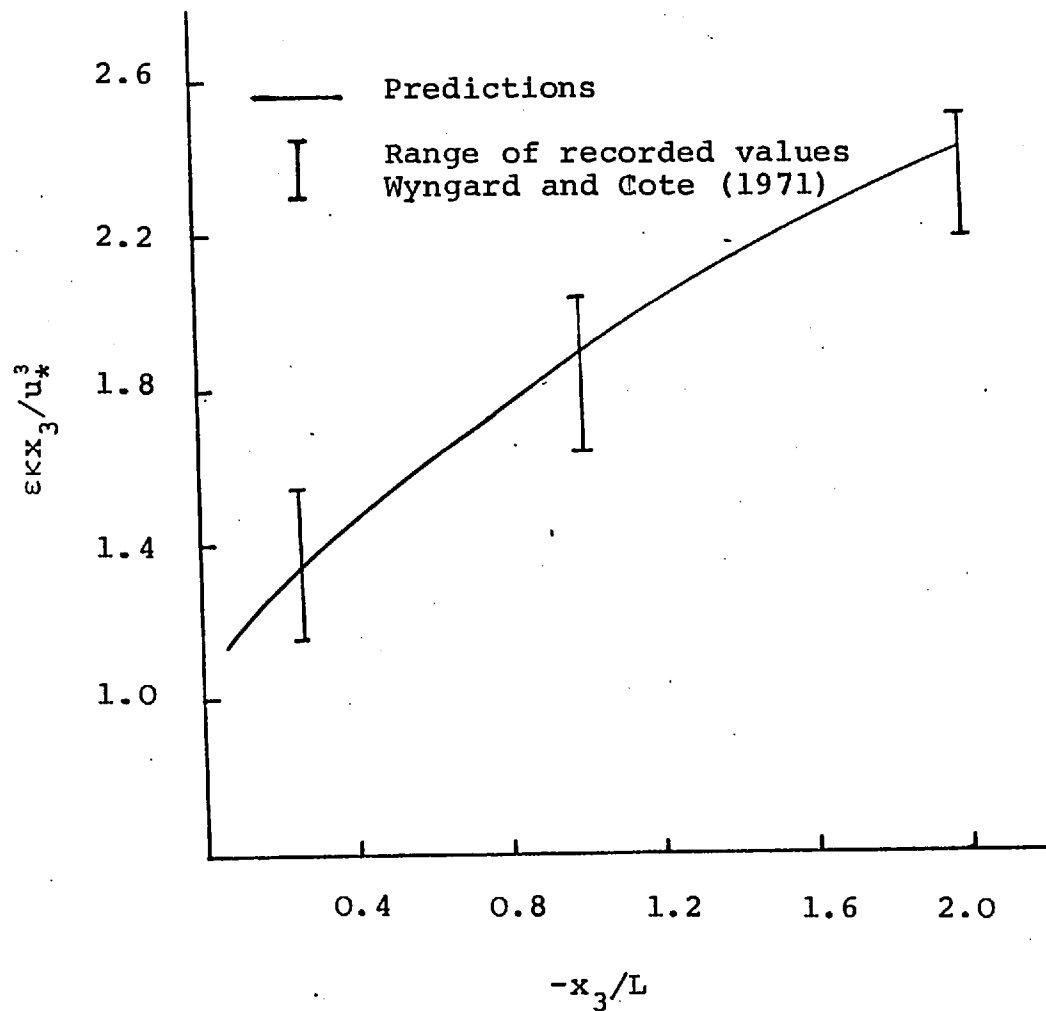


Figure 6.16 Dependence of normalised dissipation rate on unstable stratification

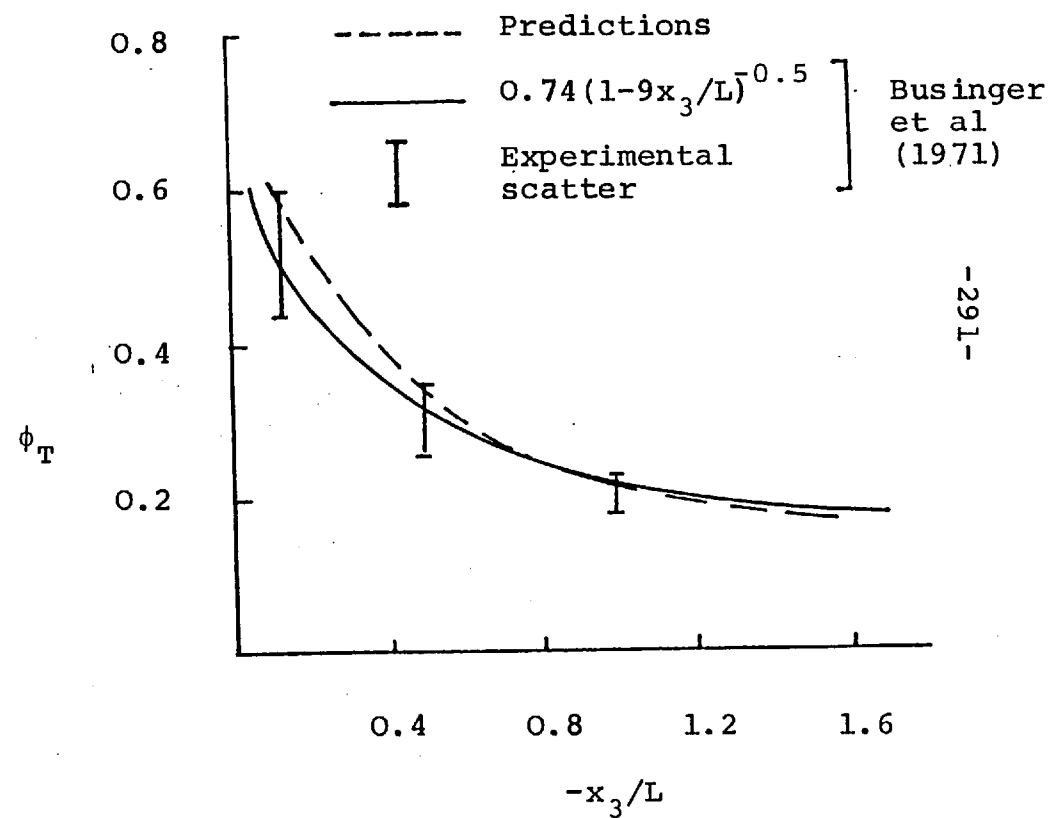


Figure 6.17 Effect of unstable stratification on normalised temperature gradient

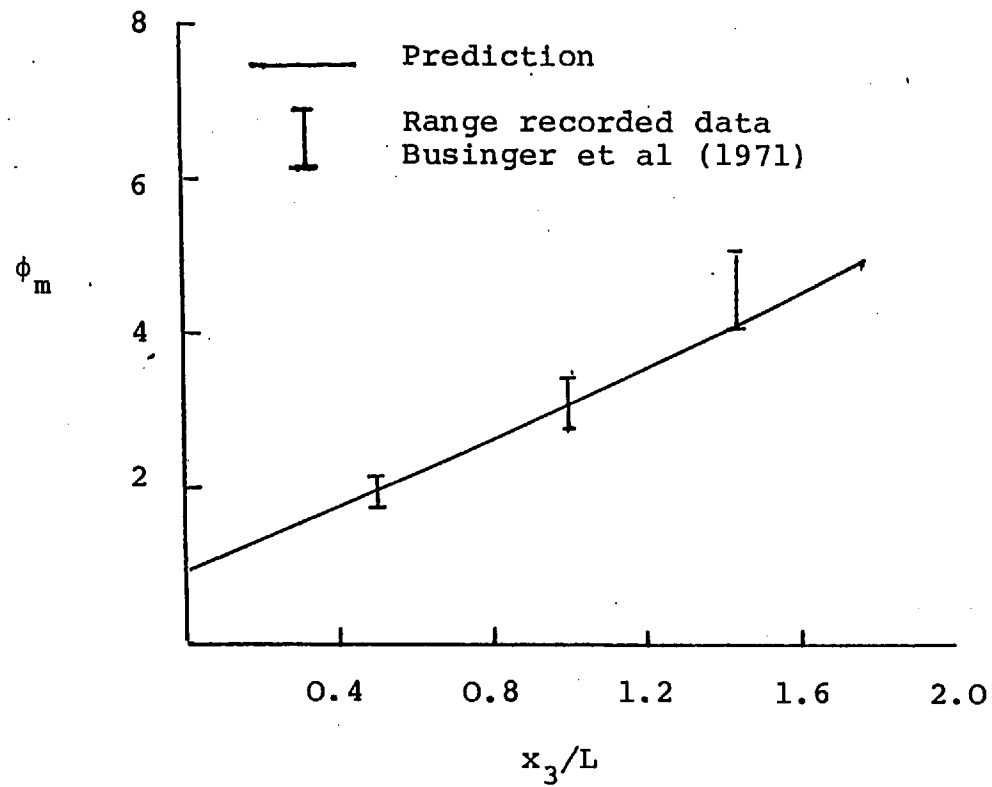


Figure 6.18 Effect of stable stratification on normalised velocity gradient

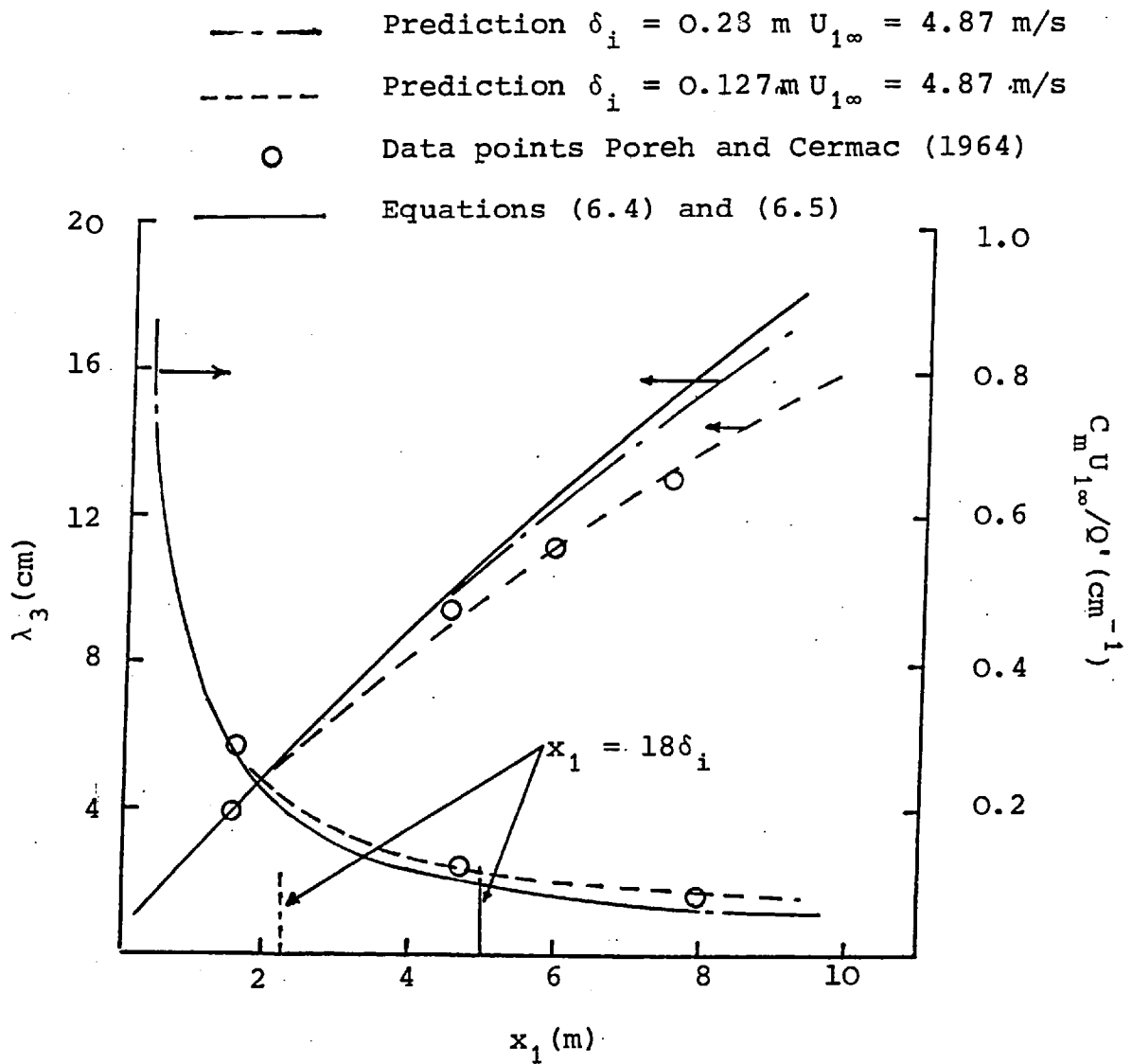


Figure 6.19 Variation of width and maximum concentration with downstream distance of a ground-level line source plume

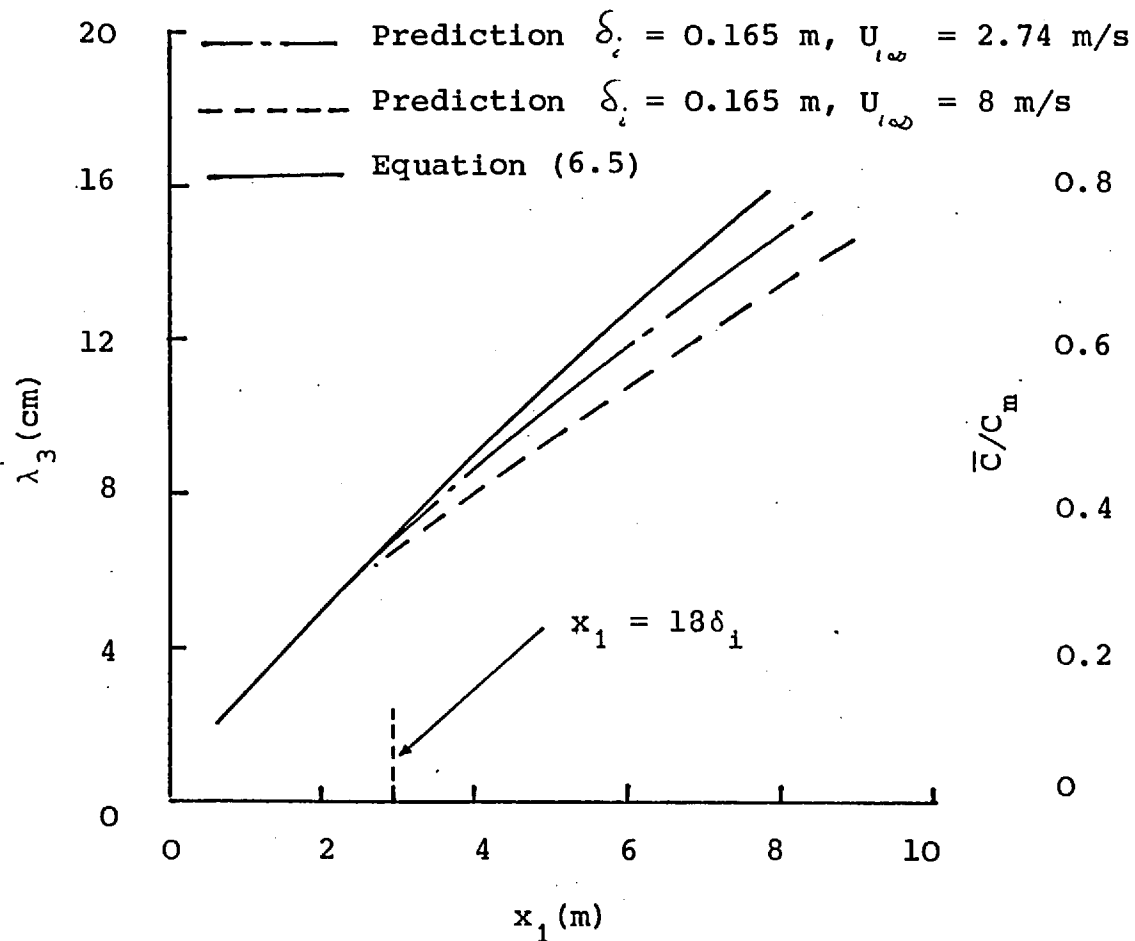


Figure 6.20 Effect of free stream velocity on width of a ground release line source plume

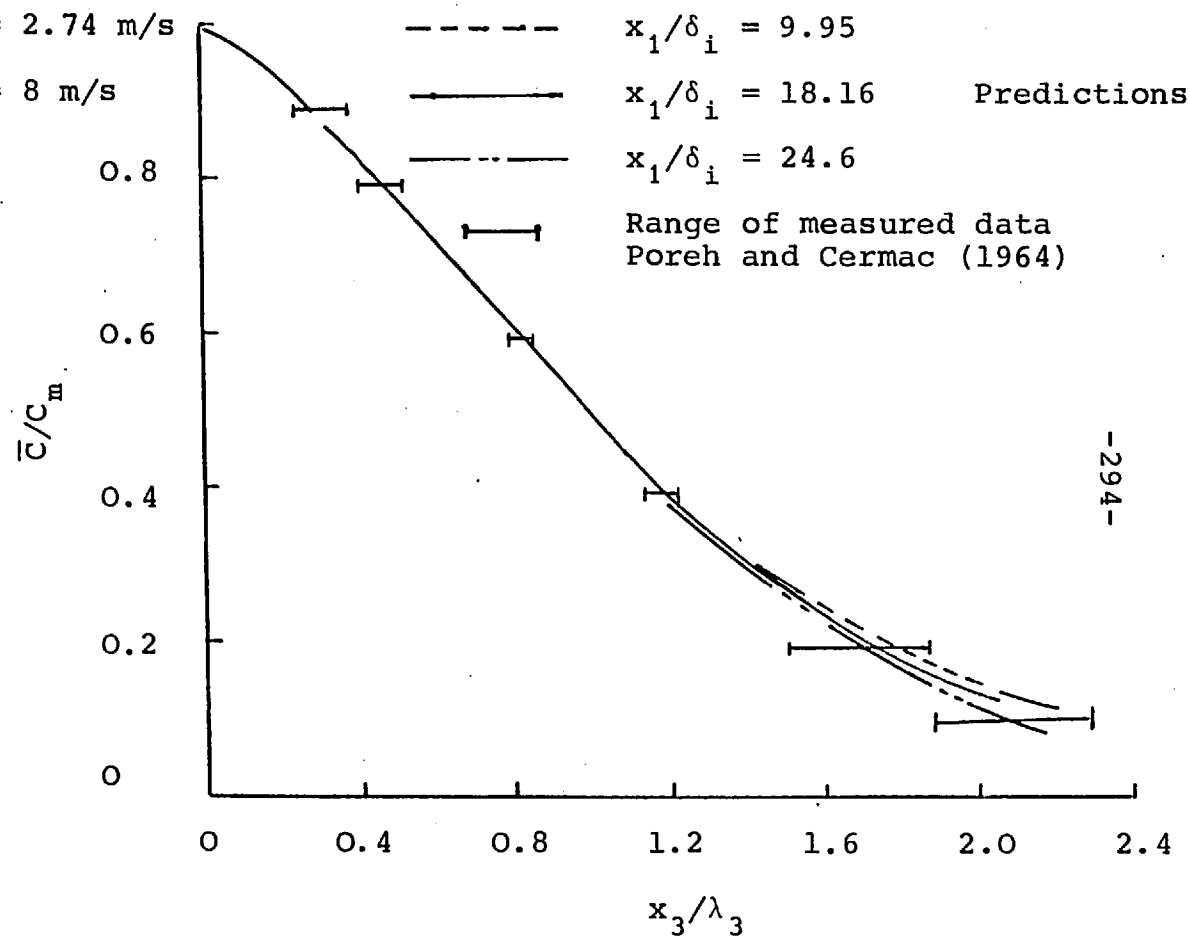


Figure 6.21 Normalised concentration profiles at different downstream stations of a ground release line source plume

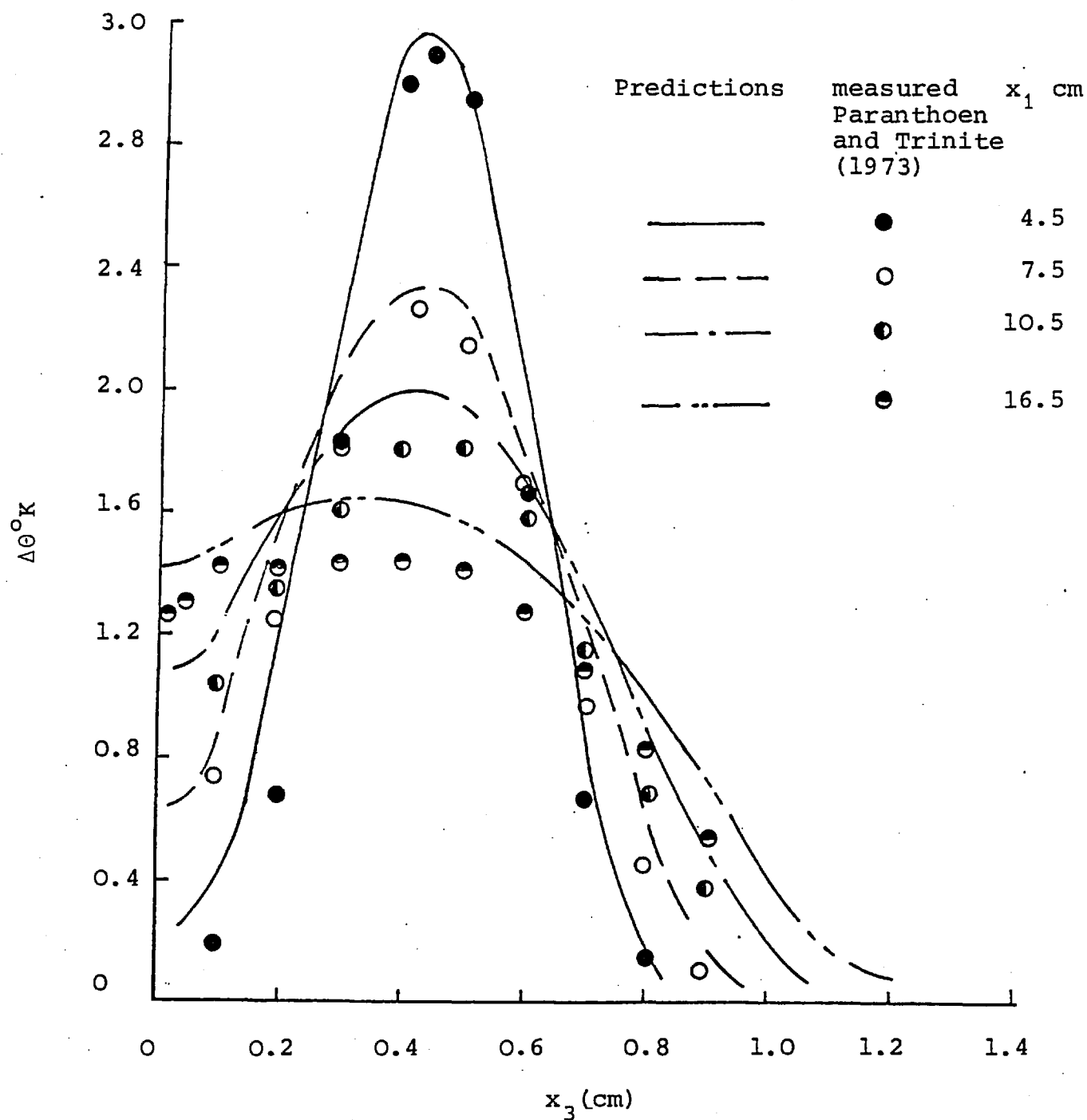


Figure 6.22 Temperature profiles for an elevated line source plume at different downstream locations

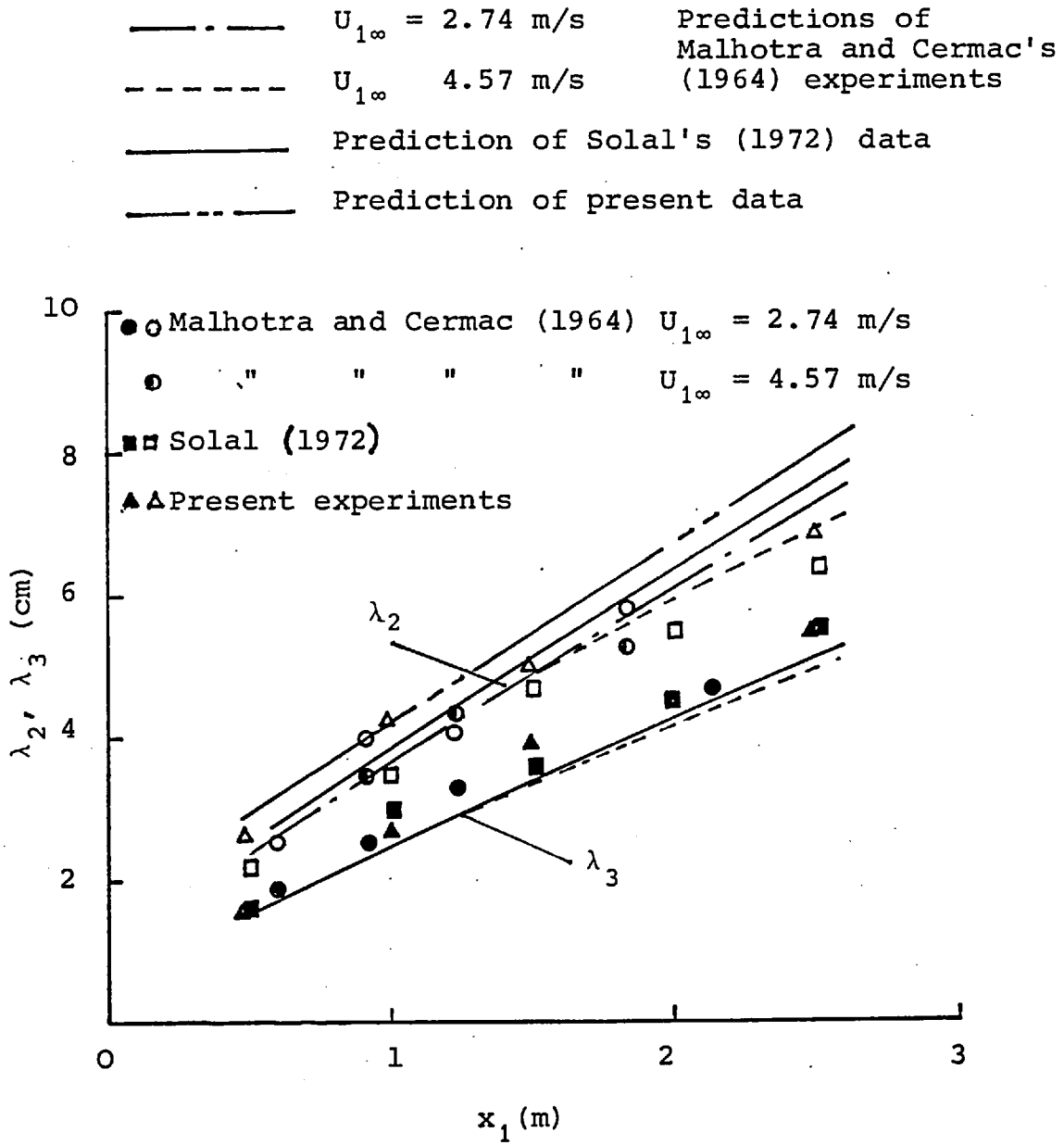


Figure 6.23 Growth of half-widths of ground level point sources

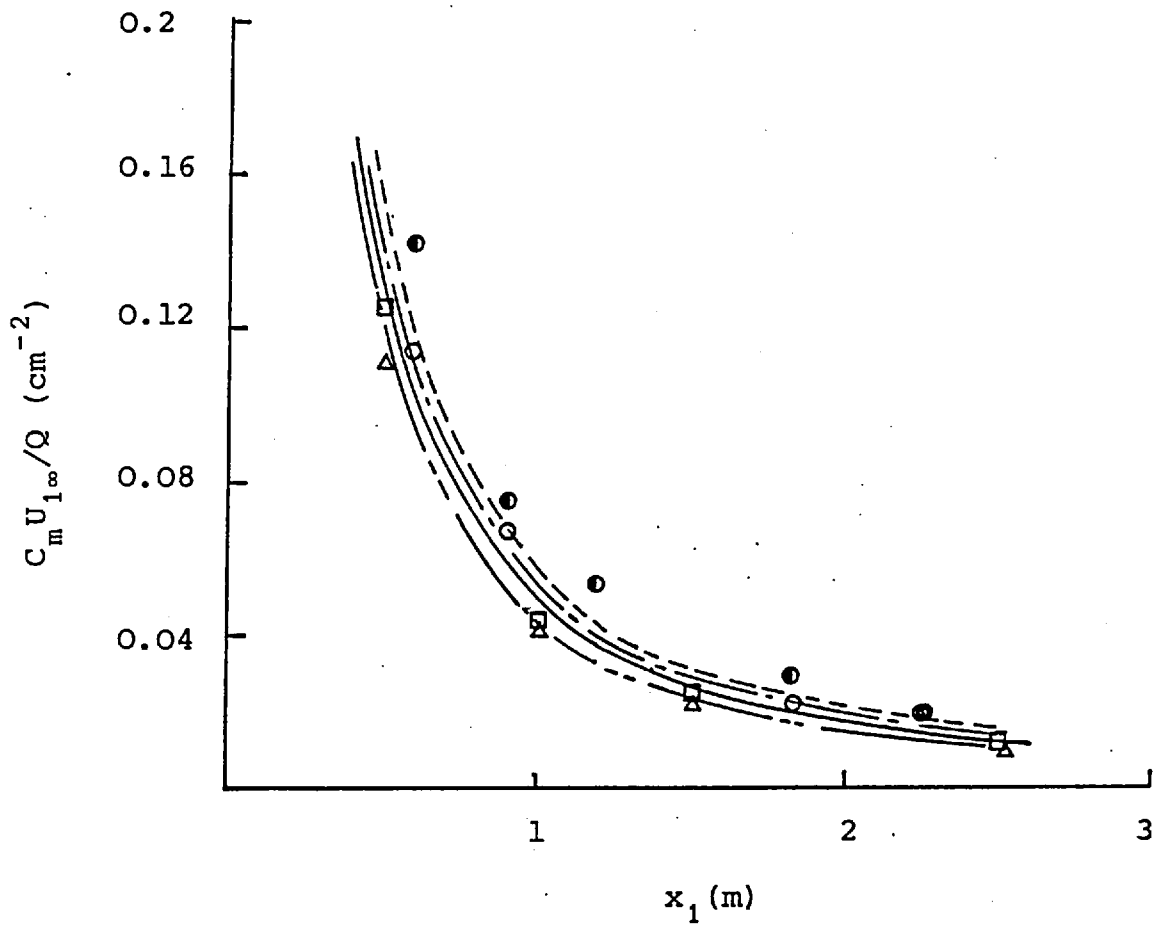


Figure 6.24 Decay of maximum concentration in ground level point source plume (for legend see Figure 6.23)

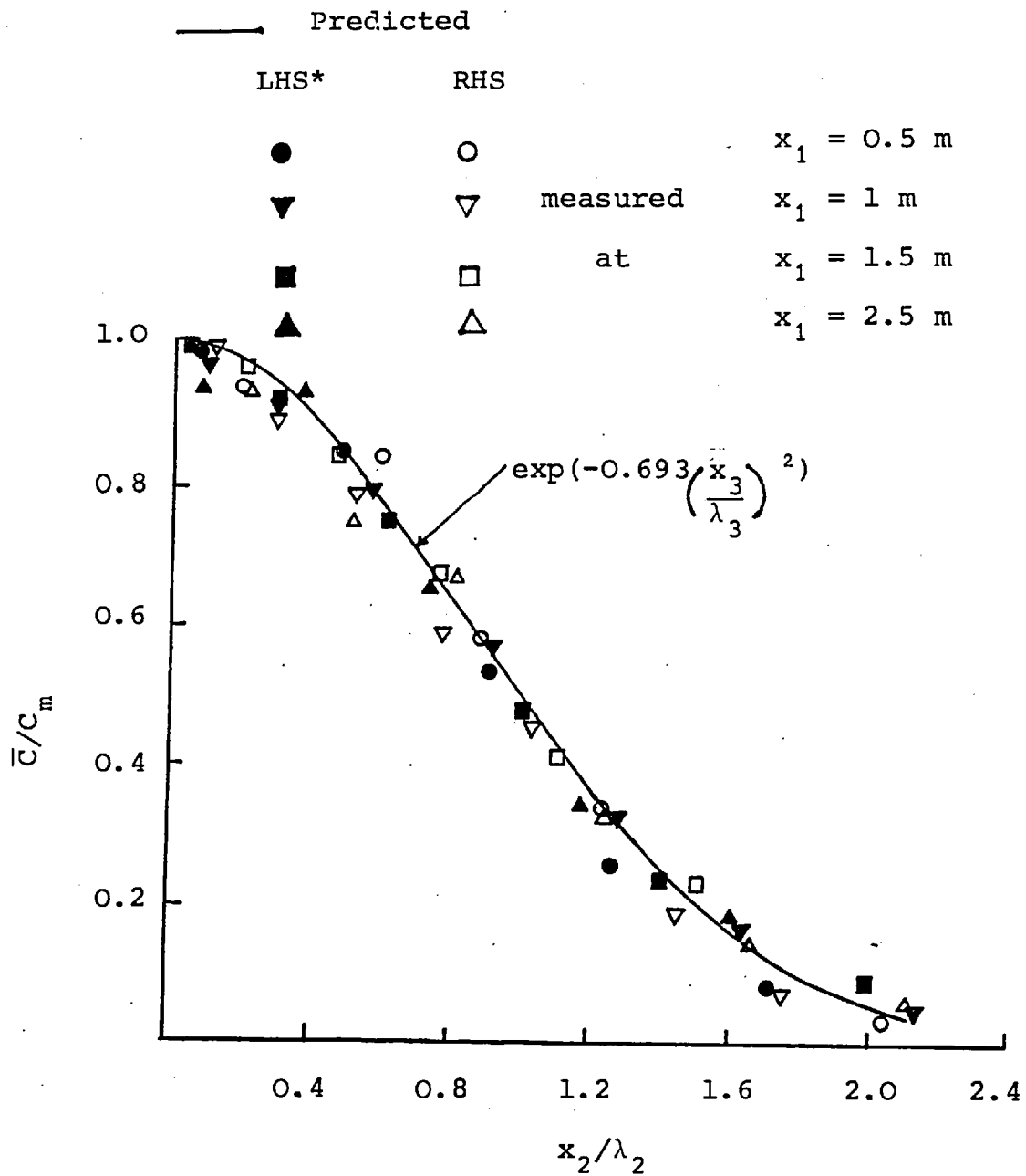


Figure 6.25 Lateral concentration profiles at different values of x_1 and $x_3 \approx 0$ for a ground release point source

*LHS and RHS refer to measurements made in the left hand side and right hand side of the plume axis when viewed in the up-stream direction.

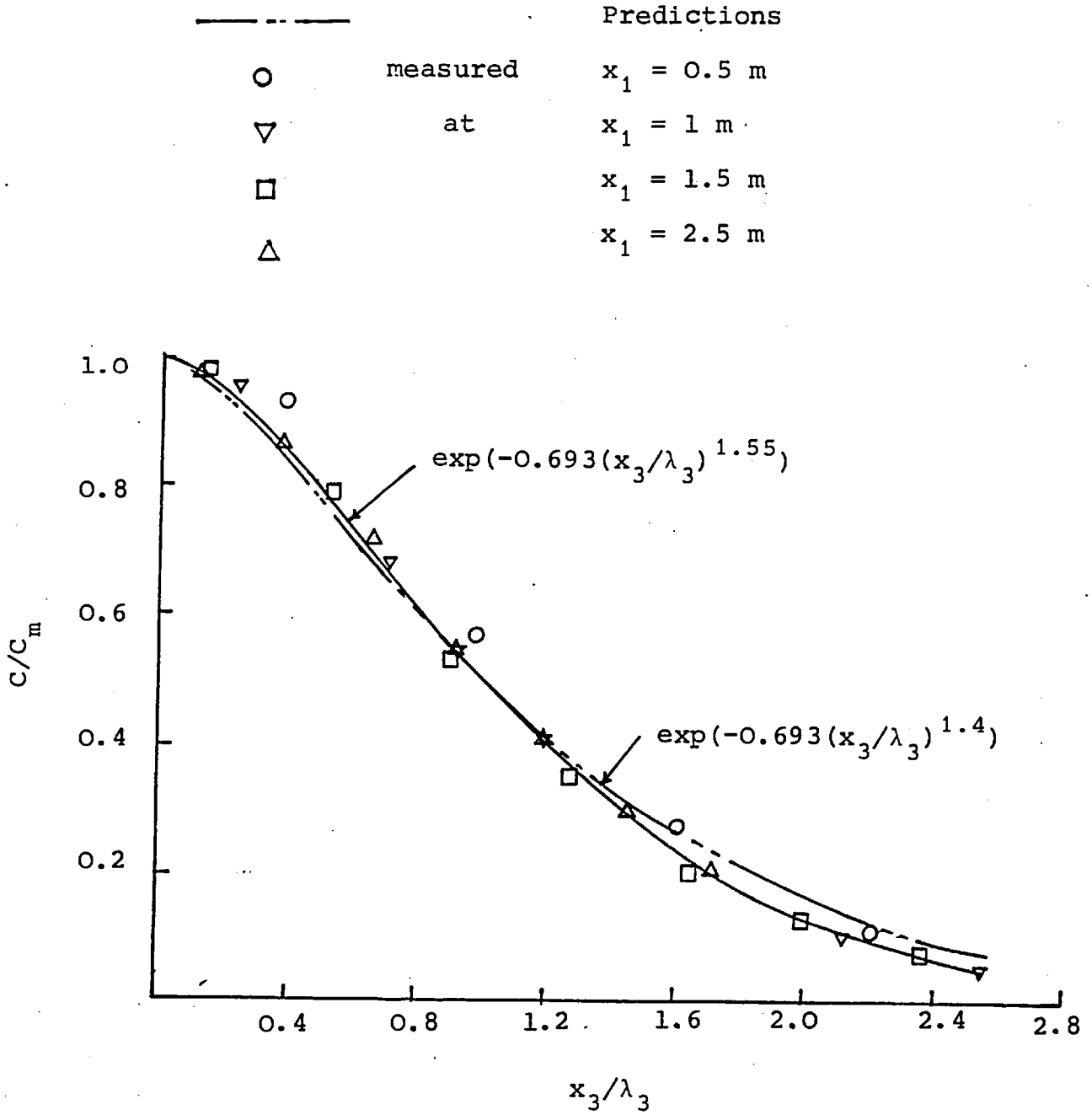


Figure 6.26 Vertical concentration profiles at different values of x_1 for a ground level point source

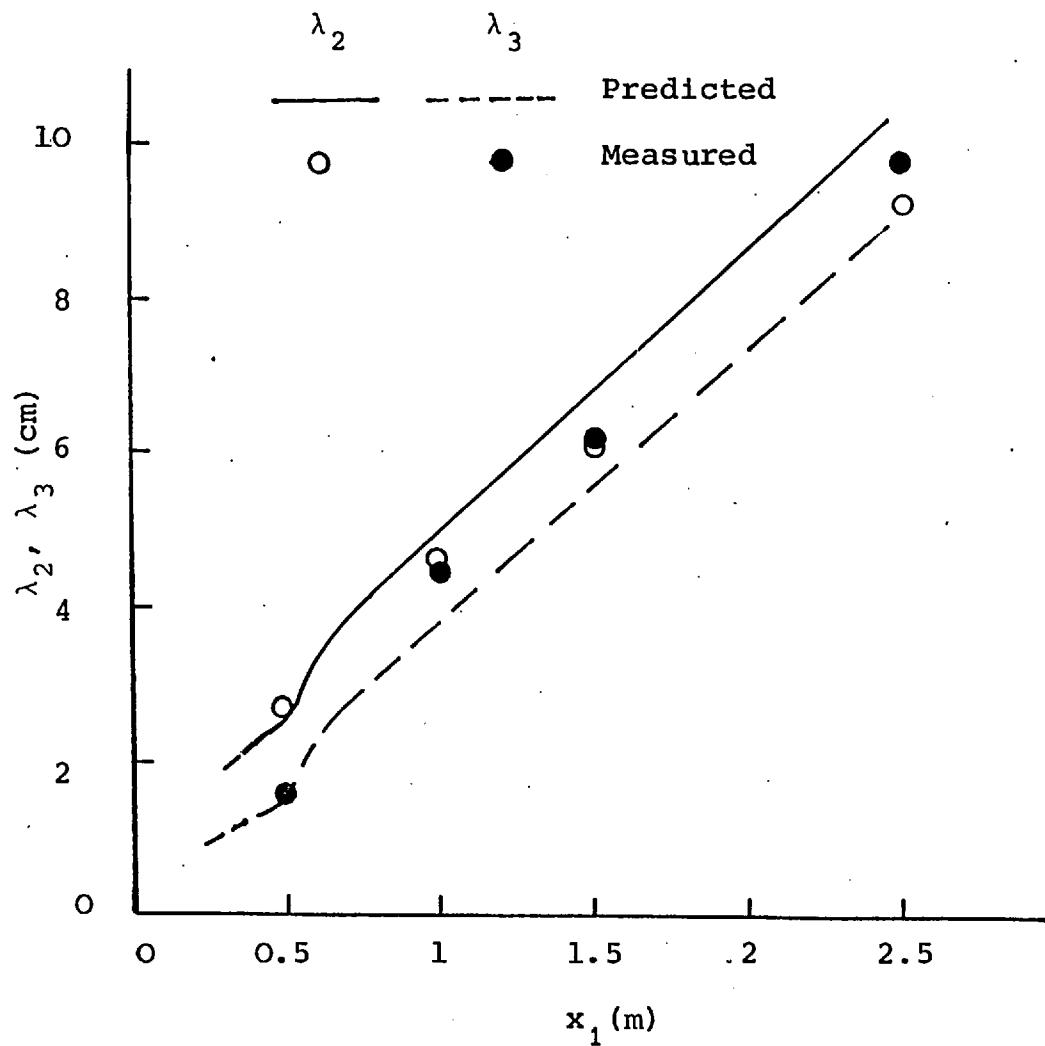


Figure 6.27 Growth of vertical and lateral spread of a ground release point source plume encountering a step change in surface roughness

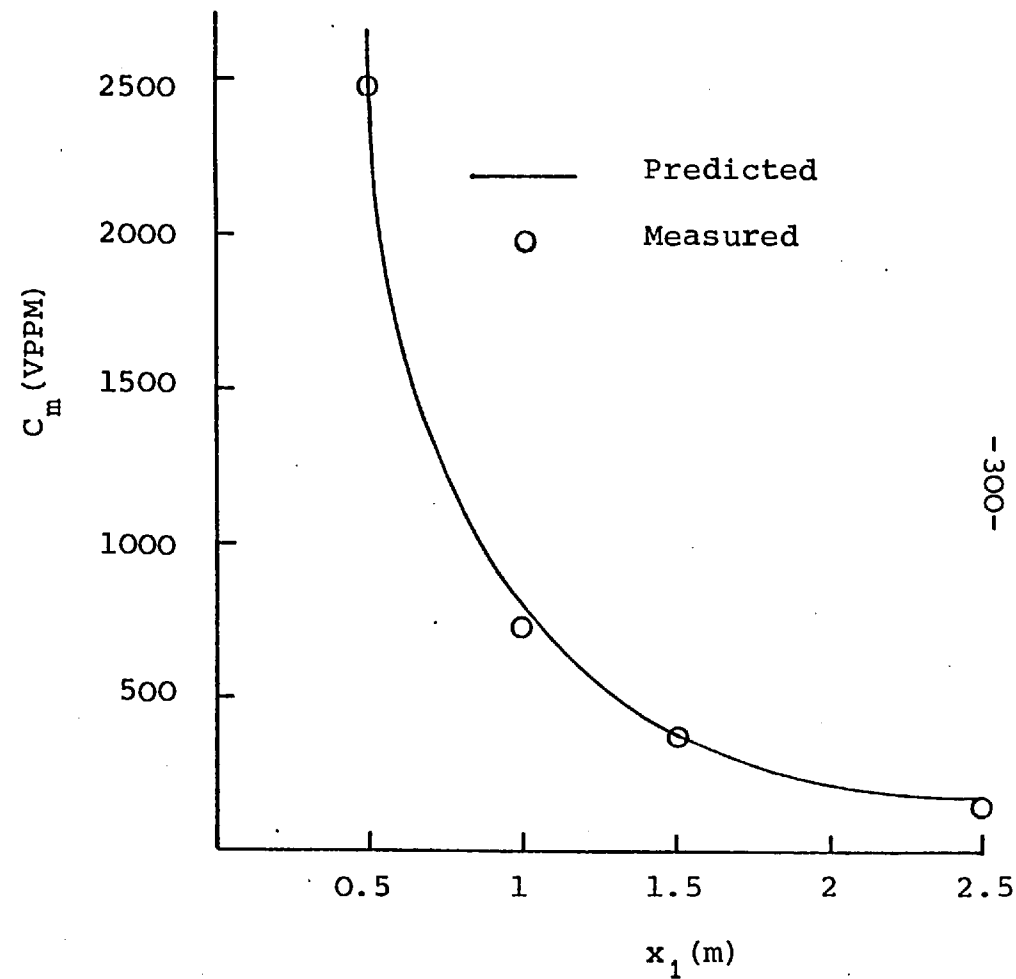


Figure 6.28 Decay of maximum concentration in a ground release point source plume encountering a step change in surface roughness

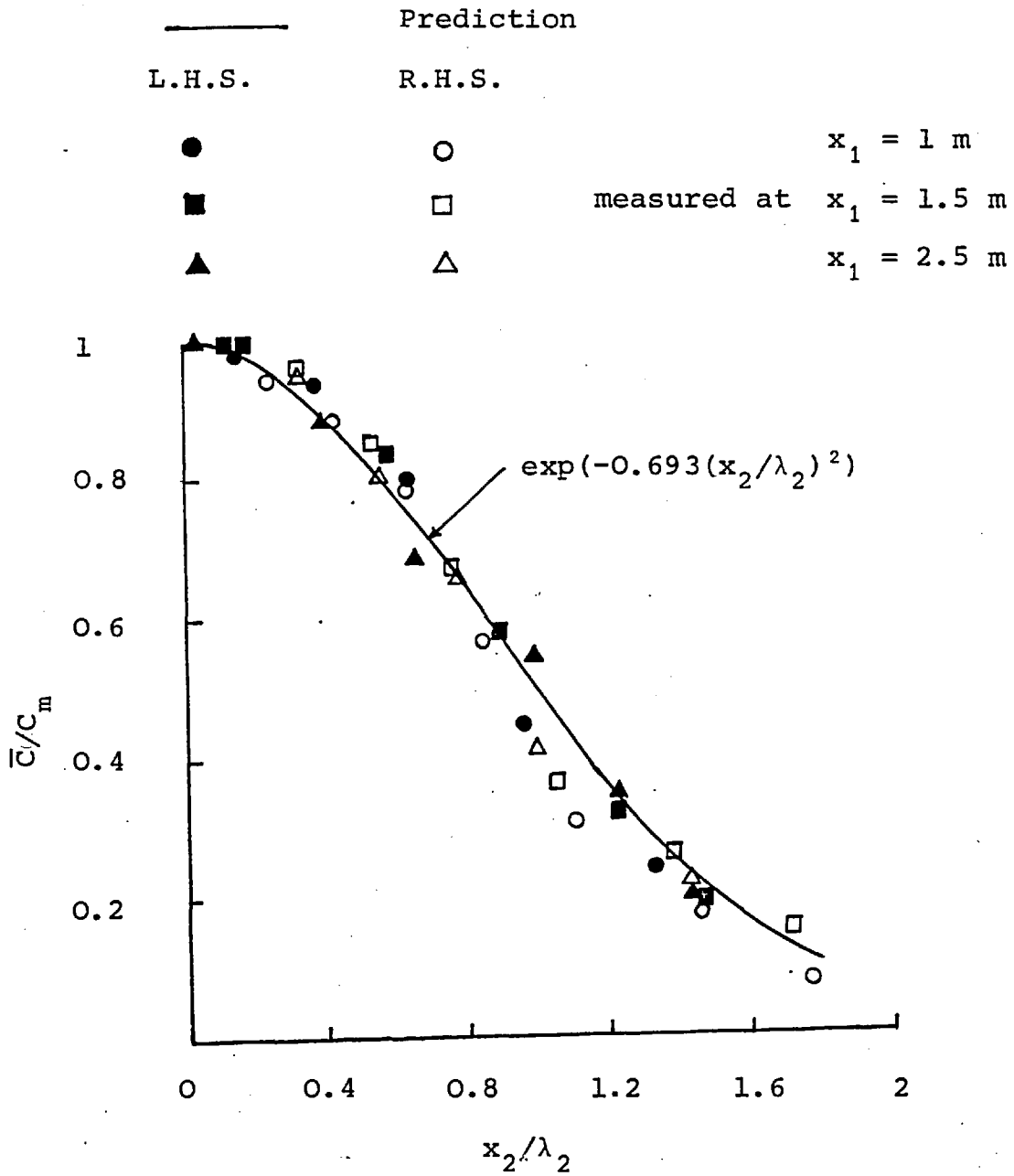


Figure 6.29 Lateral concentration profiles at different values of x_1 and $x_3 \approx 0$ of a ground release point source plume encountering a change in surface roughness

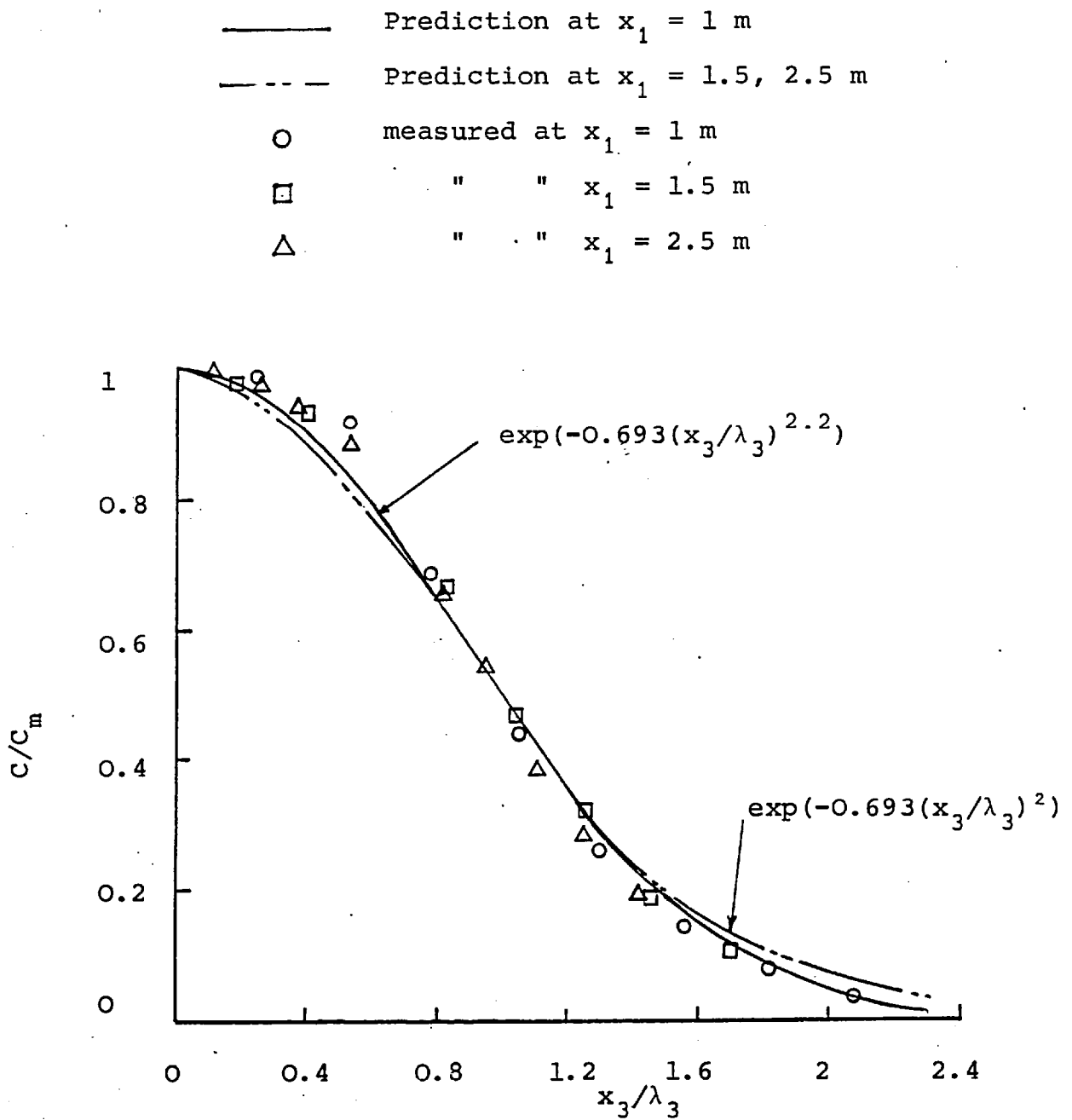


Figure 6.30 Vertical concentration profiles at different values of x_1 of a ground release point source plume encountering a change in surface roughness

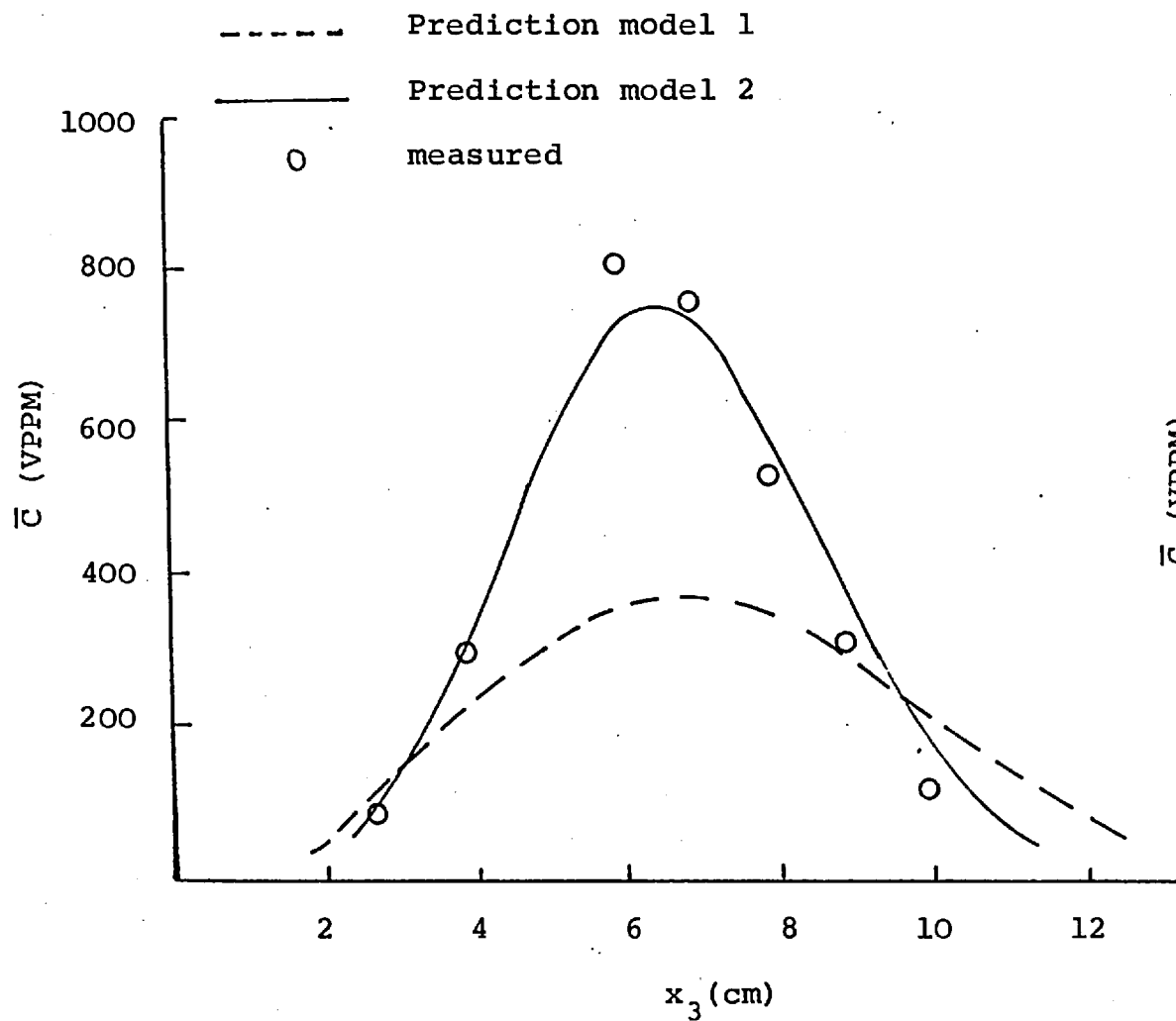


Figure 6.31 Vertical concentration profile at $x_1 = 0.5$ m and $x_2 = 0$ for an elevated point source

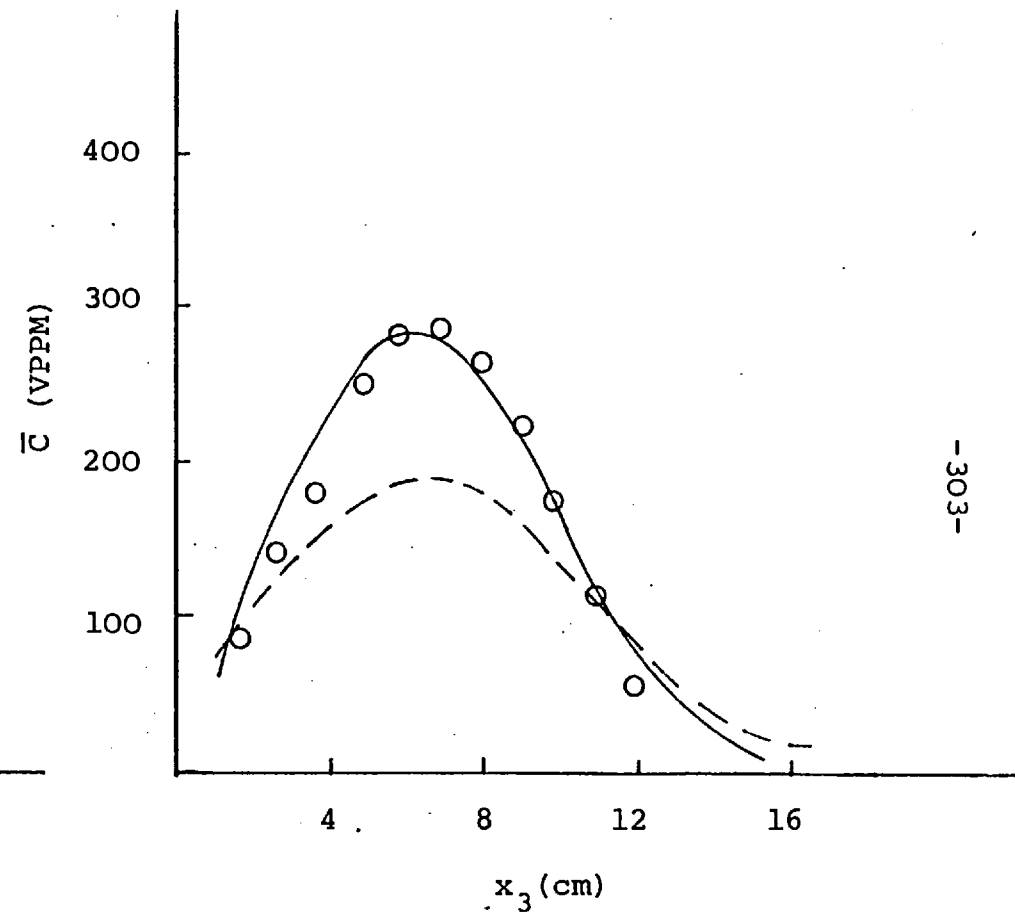


Figure 6.32 Vertical concentration profile at $x_1 = 1$ m and $x_2 = 0$ for an elevated point source (legend same as in Figure 6.31)

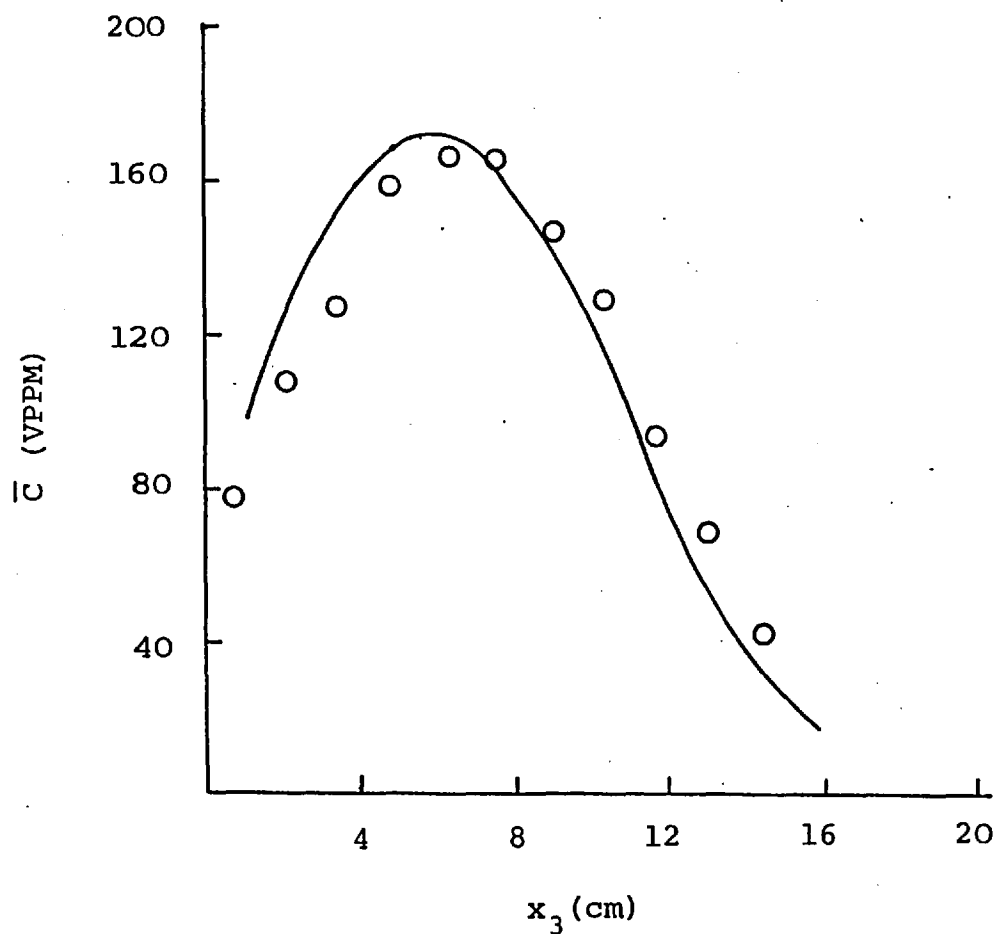


Figure 6.33 Vertical concentration profile at $x_1 = 1.5$ m and $x_2 = 0$ for an elevated point source (legend same as in Figure 6.31)

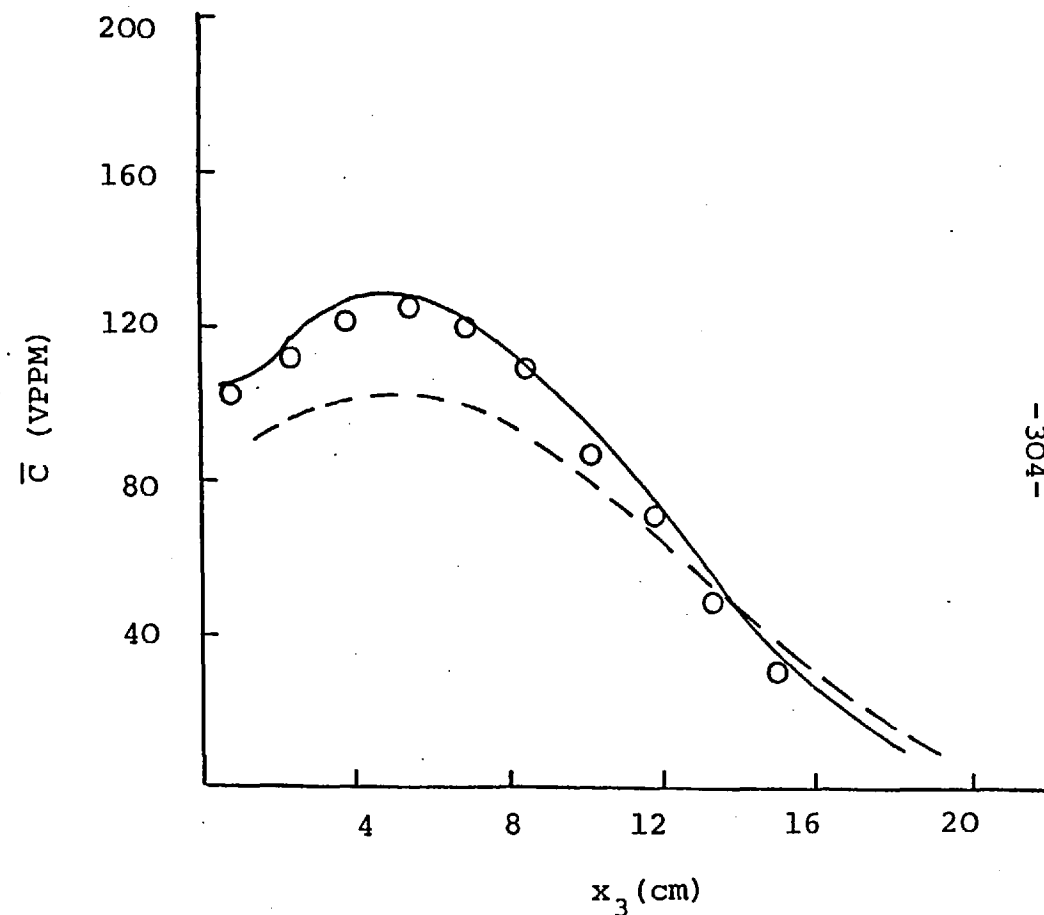


Figure 6.34 Vertical concentration profile at $x_1 = 2$ m and $x_2 = 0$ for an elevated point source (legend same as in Figure 6.31)

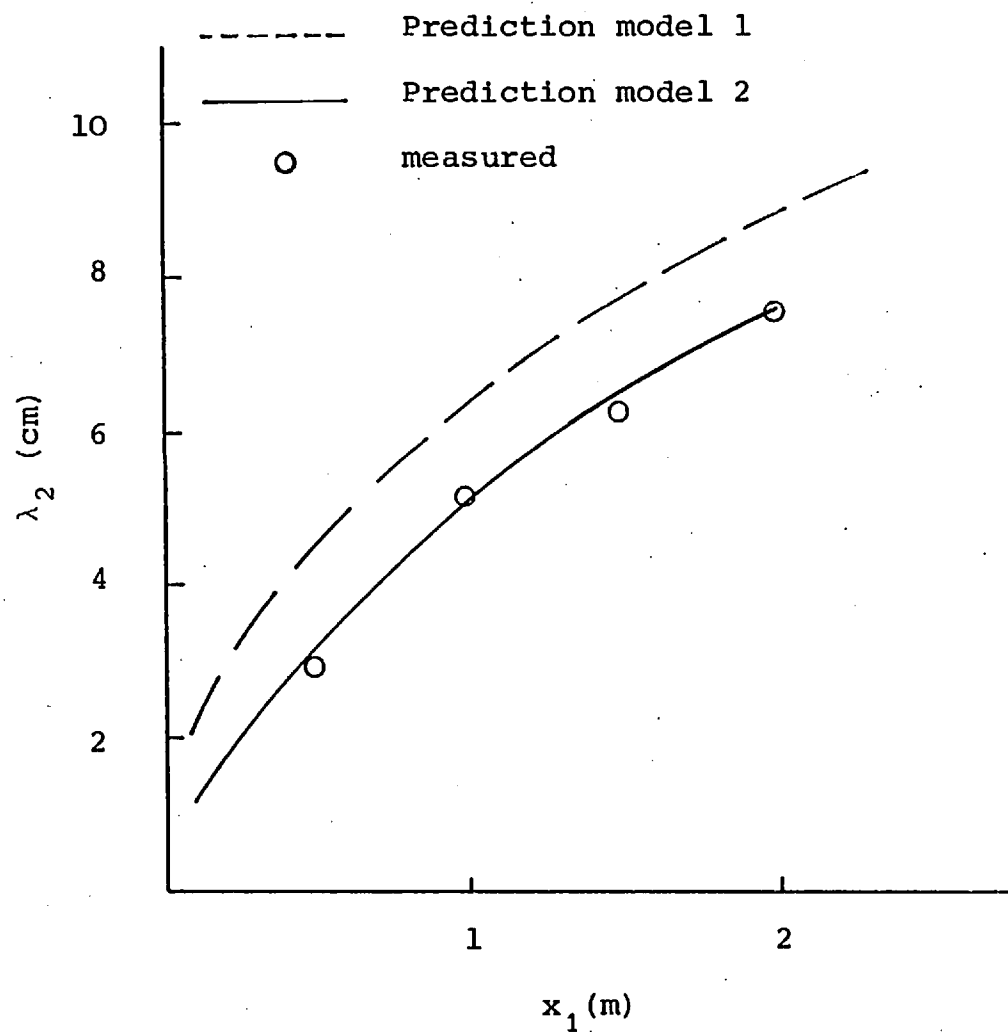


Figure 6.35 Lateral spread for an elevated point source

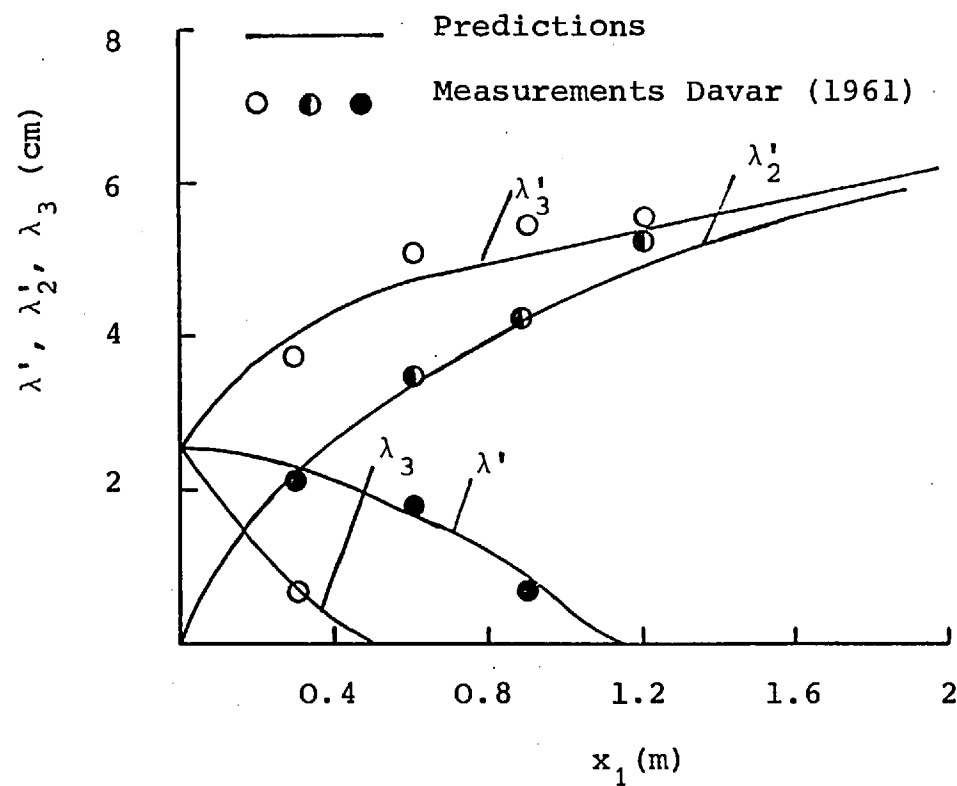


Figure 6.36 Variation of λ' , λ'_2 and λ_3 with downstream distance for an elevated point source

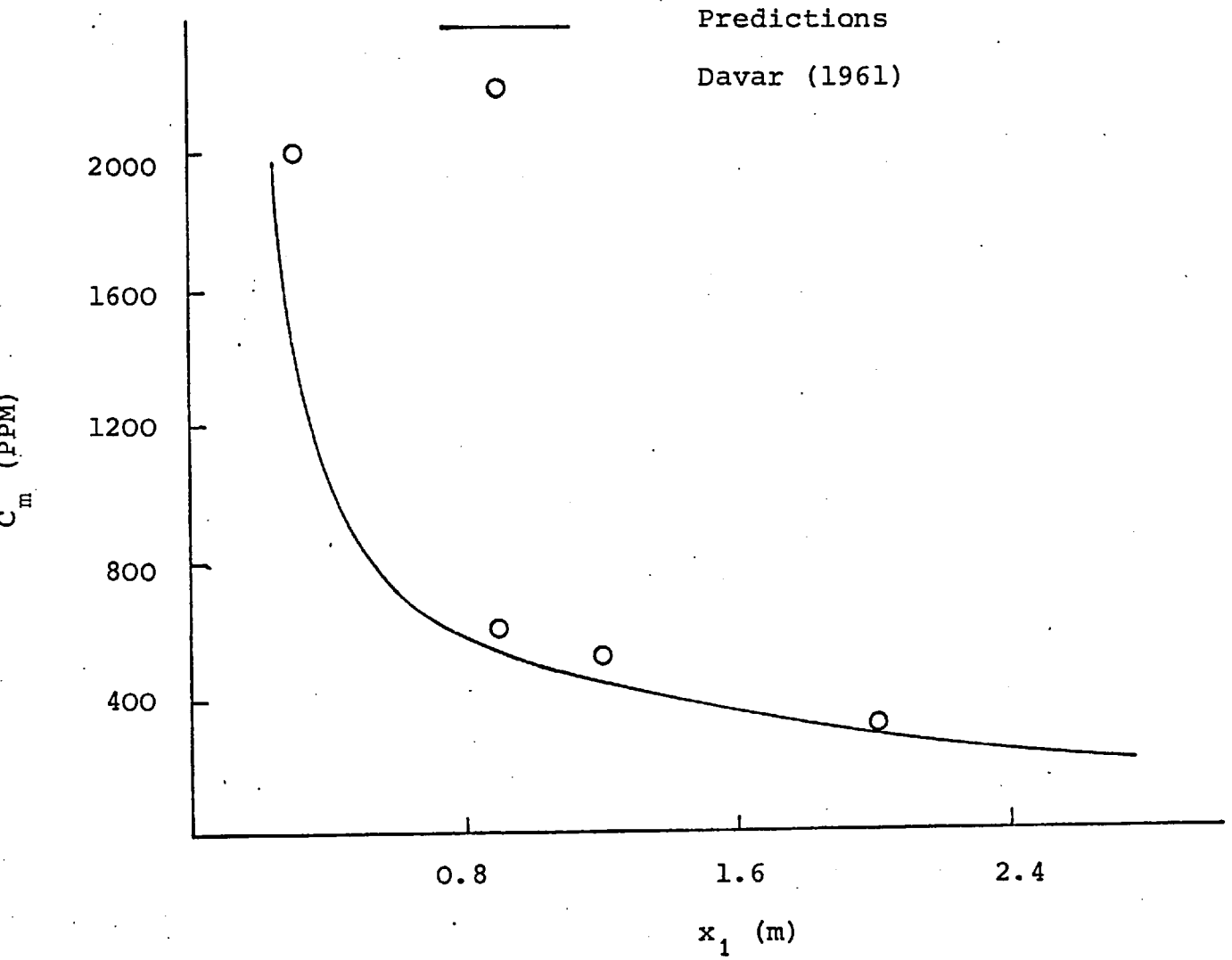


Figure 6.37 Variation of maximum concentration with x_1 for an elevated point source

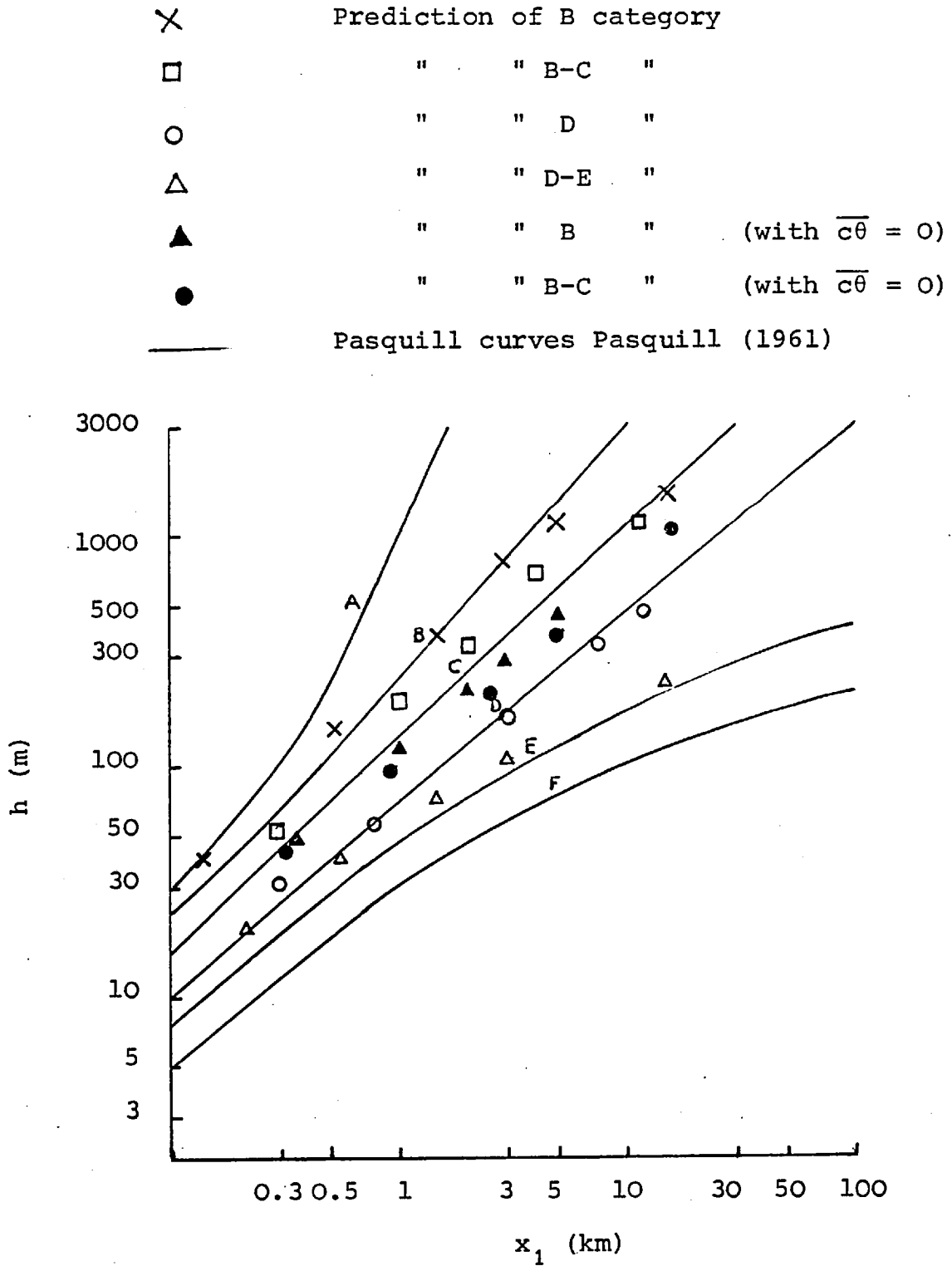


Figure 6.38 Variation of vertical spread h with x_1 for different stability categories for a ground release point source in the atmospheric boundary layer

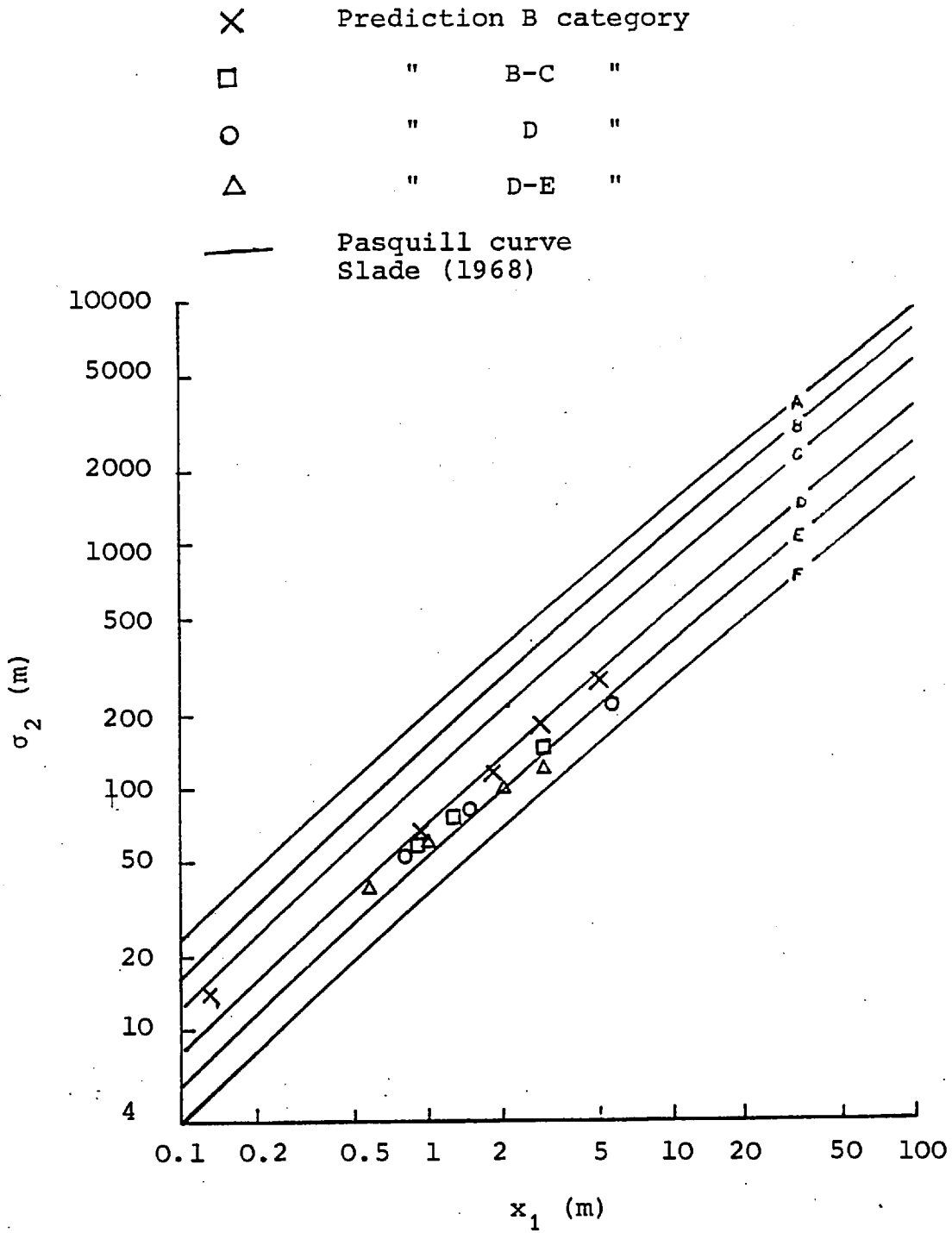


Figure 6.39 Variation of lateral spread σ_2 different stability categories for a ground release point source in the atmospheric layer