IMPROVED MATHEMATICAL TECHNIQUES
FOR SOLUTION OF
ATMOSPHERIC DISPERSION MODELS

A Dissertation

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by

Miguel T. Fleischer

March, 1978

To

My lovely wife, Jackie

and to

David and Ronnie

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CHAPTER I

INTRODUCTION

The increasing cost of controlling emissions from industrial sources has magnified the need to develop accurate mathematical models which can relate emission rate to air quality. In order to adequately describe the relationship between emissions and air quality, a model must be able to describe the variable (time and space) meteorological parameters and the chemical or physical processes which remove pollutants from the atmosphere.

During the past years, several models have been presented in the literature [8], ranging from very simple ones like the box model to more general cases solved by finite-difference techniques. The Eulerian formulation [8] has been the most common approach due to the availability of numerical techniques with which the equations can be solved.

A general model, one which includes temporal and spatial variations of meteorological parameters, should provide a good description of atmospheric diffusion processes. A dispersion model based on the K-theory and solved using orthogonal collocation was presented by Fleischer [8]. The atmospheric processes were described by the 3-dimensional, unsteady-state diffusion equation including chemical reactions. The work was validated with existing experimental data and shown to have several significant advantages over other available methods.

Understanding of the cause-effect relationship of pollutant emission and dispersion on the air quality may be difficult through a complex general air pollution model. In addition, analytical solutions are available only for simplified diffusion equations. The disadvantages of solving simple cases using the same complex general method gave rise to the present work.

Dispersion models based on the K-theory and solved by improved mathematical techniques using spline orthogonal collocation are presented. All types of steady-state air pollution problems are simulated. These models extend from the simple ground level line source case to the complex 3-dimensional elevated point source model including the Coriolis effect. Spline orthogonal collocation, a weighted residual method, reduces the partial differential equation governing the mean concentration of pollutant species, within the plume generated by the source, to first-order ordinary differential equations. This system of equations is solved in a digital computer.

The present work was evaluated by comparing the results to available analytical solutions, e.g., two or three-dimensional cases with constant turbulent diffusivities and mean wind velocity, and no reaction. Mathematical parameters, inherent of the techniques developed, are determined through parametric studies. In addition, several hypothetical cases are simulated to explore the present method response to variations in atmospheric conditions.

CHAPTER II

FORMULATION OF MODELS AND THEIR SOLUTION TECHNIQUES

The basic mathematical statement for description of the temporal and spatial distribution of chemical species by the Eulerian approach is the mass balance or continuity equation. This equation, applied to a single species in the atmosphere, based on the K-theory is:

$$\frac{\partial C}{\partial t} + u\,\frac{\partial C}{\partial x} + v\,\frac{\partial C}{\partial y} + w\,\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}(K_x\,\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(K_y\,\frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(K_z\,\frac{\partial C}{\partial z}) + R \qquad (2.1)$$

The main objective of the present work is to predict the concentration distribution with respect to time and space for various atmospheric dispersion cases. The diffusion equation (2.1) is the basis for all the models presented here. A description of these models and their methods of solution is given next, starting with the simplest one, the two dimensional continuous ground level line source.

Two Dimensional-Continuous Ground Level Line Source

A widely studied situation is the case of an infinite line source in the y-direction at ground level emitting at a constant rate. At steady state, equation (2.1) is simplified as

$$\frac{\partial C}{\partial t} = 0 \qquad (2.2)$$

In addition, for an infinite crosswind (y) line source,

$$\frac{\partial}{\partial y}(K_y\,\frac{\partial C}{\partial y}) = 0 \qquad (2.3)$$

Upon assuming that the mean flow is along the x-axis, i.e.,

$$v = w = 0 \tag{2.4}$$

and that the diffusion in the x-direction is negligible compared to the transport by the mean flow, i.e.,

$$\frac{\partial}{\partial x}(K_x \frac{\partial C}{\partial x}) << u \frac{\partial C}{\partial x} \tag{2.5}$$

equation (2.1) for the case when no chemical reactions are included, i.e., R=0 reduces to

$$u \frac{\partial C}{\partial x} = \frac{\partial}{\partial z}(K_z \frac{\partial C}{\partial z}) \tag{2.6}$$

with boundary conditions

$$C \to 0 \qquad \text{as} \qquad x,z \to \infty \tag{2.7a}$$

$$C \to \infty \qquad \text{at} \qquad x = z = 0 \tag{2.7b}$$

$$K_z \frac{\partial C}{\partial z} \to 0 \qquad \text{as} \qquad z \to 0,\ x > 0 \tag{2.7c}$$

The last boundary condition implies zero flux at the surface, i.e., the pollutant is completely reflected.

For the lower atmosphere, in adiabatic conditions, it has been seen that the wind velocity varies with the logarithm of the height. However, such a functional relationship proves intractable if an analytical solution of equation (2.6) is desired. When a power-law form is adopted for both the mean wind and turbulent diffusivity profiles, i.e.,

$$u = u_1 (\frac{z}{z_1})^m \qquad\qquad K_z = K_1 (\frac{z}{z_1})^n \tag{2.8}$$

the analytical solution [2], valid for $r = m-n+2 > 0$, is

$$C(x,z) = \frac{Qr}{u_1\Gamma(s)}\left[\frac{u_1}{r^2K_1x}\right]^s \exp\left(-\frac{u_1z^r}{r^2K_1x}\right) \tag{2.9}$$

where $s = \frac{m+1}{r}$ and z_1 is taken to be unity.

Continuity should be satisfied at any position in the x(downwind) direction:

$$\int_0^\infty u\, C(x,z)dz = Q \qquad \text{for all} \qquad x > 0 \tag{2.10}$$

where Q is the constant emission rate per unit crosswind length.

The case which is solved in the present work considers m=n=0, i.e., the diffusion is Fickian. Equation (2.6) becomes

$$u\,\frac{\partial C}{\partial x} = K_z\,\frac{\partial^2 C}{\partial z^2} \tag{2.11}$$

and the analytical solution is reduced to

$$C(x,z) = \frac{2Q}{u\sqrt{\pi}}\left[\frac{u}{4K_zx}\right]^{\frac{1}{2}} \exp\left[-\frac{uz^2}{4K_zx}\right] \tag{2.12}$$

The boundary condition $C \to 0$ as $z \to \infty$ is too restrictive because it cannot be applied to a case with an inversion layer at a certain height. This situation can be represented by

$$K_z\,\frac{\partial C}{\partial z} = 0 \qquad \text{at} \qquad z = z_{max} \tag{2.13}$$

Therefore, equation (2.13) is used as the second boundary condition in the vertical direction. If a comparison with the analytical solution is desired, z_{max} can be given a sufficiently large value such that the pollutant never reaches the inversion layer. In addition, a solution is usually needed up to a definite position in the x-direction. Equation (2.11) is solved numerically for

$$0 < x \leq x_{max} \qquad ; \qquad 0 \leq z \leq z_{max} \tag{2.14}$$

A transformation of the spatial coordinates to yield limits of 0 to 1 is performed by using

$$\xi = \frac{x}{x_{max}} \qquad\qquad z^* = \frac{z}{z_{max}} \tag{2.15}$$

To complete the problem, a boundary condition in the x-direction must be specified, and the constant emission rate taken into account.

The model by Fleischer [8] defined the location of the source through a boundary condition in the x-direction as

$$C = \begin{cases} C_o & \text{at} \qquad x = 0 \\ 0 & \text{elsewhere} \end{cases} \tag{2.16}$$

where C_o is an equivalent source concentration to be calculated from the emission rate using quadrature weights. Orthogonal collocation was the numerical technique used for solving the partial differential equation (2.1). One of the reasons as to why this was done is the attractive feature of being able to position the point source exactly as a collocation point with concentration C_o and the rest of the collocation points at x=0 with zero concentration. However, this procedure gives rise to several problems:

1) Global collocation must be used, i.e., collocate points to reduce the partial differential equation to a system of ordinary differential equations throughout the entire region of interest. Since the

solution to a dispersion model should have approximately the shape of a conical plume, only a few points would be within this region. This means that at several positions in the x-direction, especially close to the source, only some points would have a certain concentration value and the rest would contain zero concentration. Accurate interpolation from such a concentration distribution is impossible;

2) One of the collocation points must match the location of the source; and

3) A ground level source cannot be placed at z=0, but at the position of the first collocation point, since only interior collocation points are used in the solution.

In spite of all these restrictions, which will be removed in the present work, it was proven that orthogonal collocation has better properties than other numerical techniques, and therefore will be used here again.

A point source, which usually represents a stack, can be considered as a very small area normal to u with a concentration C_o equivalent to the constant emission rate, as shown in Figure 2.1.

The present model then will have a discontinuous initial value profile expressed as

$$C^i = \begin{cases} C_o & \text{at} \quad \xi=0 \quad , \quad 0 \le z^* \le \beta \\ 0 & \text{at} \quad \xi=0 \quad , \quad z^* > \beta \end{cases} \tag{2.17}$$

where C_o can be calculated using equation (2.10):

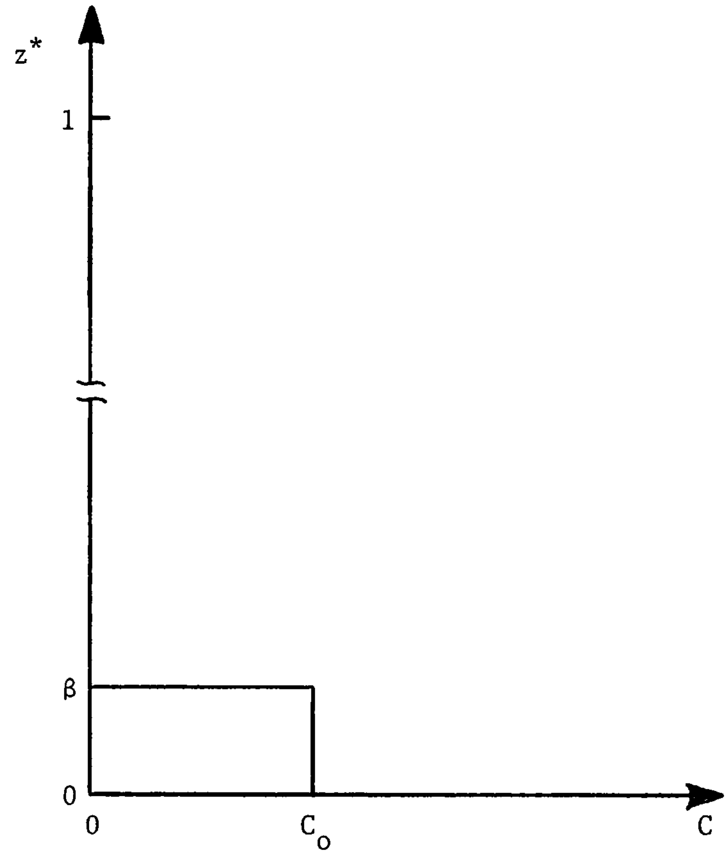

FIGURE 2.1 VERTICAL CONCENTRATION DISTRIBUTION AT x=0 - GROUND LEVEL LINE SOURCE

$$Q = \int_o^\beta uC_o z_{max} dz^*$$

Solving for C_o:

$$C_o = \frac{Q}{u\ \beta\ z_{max}} \qquad (2.18)$$

Determination of the concentration distribution as a function of the spatial variables x and z requires then the solution of equation (2.11) with boundary conditions given by (2.7c) and (2.13), and the initial condition given by (2.17). The way this model is formulated overcomes the restrictions, 2) and 3), previously discussed.

A suitable approach to this problem is immediately suggested by using spline orthogonal collocation in the vertical direction. A small interval $[\beta-\delta_1, \beta+\delta_2]$ is considered and equation (2.11) is only solved in this interval. The required variable transformation is:

$$z^* = (\delta_1 + \delta_2)\zeta + \beta - \delta_1 \tag{2.19}$$

where $0 \leq \zeta \leq 1$. Equation (2.11) remains then as,

$$R_1 \frac{\partial C}{\partial \xi} = R_5 \frac{\partial^2 C}{\partial \zeta^2} \tag{2.20}$$

where

$$R_1 = \frac{u}{x_{max}} \quad ; \quad R_5 = \frac{K_z}{z_{max}^2(\delta_1+\delta_2)^2} \tag{2.21}$$

Global orthogonal collocation is applied to the ζ domain such that a system of first order ordinary differential equations with respect to ξ is left to be solved. The zeros of the Jacobi polynomials $P_{N_z}^{(0,0)}$ serve as collocation points.

The concentration distribution is obtained only within the $[\beta-\delta_1, \beta+\delta_2]$ interval in the z^* domain, where the concentration is known to have a significant value, not just zero. Therefore, restriction 1) is eliminated from the method of solution. As x increases the penetration zone is broadened by choosing larger δ_1 and δ_2. This implies that the technique considers moving boundary conditions in the vertical direction, and the edge of the plume is known at any position along the mean wind direction.

The calculational procedure is as follows: at any integration step, the concentrations at $\zeta=0$ and $\zeta=1$ are compared with C_o and zero, respectively. If the comparisons agree, as it is shown in Figure 2.2 the values for δ_1 and δ_2 are assumed correct and the integration continues to the next step.

Since the concentrations should approach C_o and 0 at $\zeta=0$ and $\zeta=1$, respectively, the use of the following boundary conditions is valid:

$$\frac{\partial C}{\partial \zeta} = 0 \qquad \text{at} \qquad \zeta=0,\ \zeta=1 \tag{2.22}$$

If at any step, the concentration at $\zeta=0$ is considerably smaller than C_o, δ_1 is increased and the integration is performed for that same x with the previous good solution as initial condition. This comparison stops when δ_1 becomes β. When the concentration at $\zeta=1$ is considerably larger than zero, the same previous procedure is applied to δ_2. Finally, if an inversion layer is reached ($\delta_2=1-\beta$) global collocation is used to continue the calculations until $x=x_{max}$. In any problem β is usually small so that the condition $\delta_1=\beta$ will always be obtained before $\delta_2=1-\beta$.

This technique gives rise to the question as to how close to zero, the "zero concentration" is. The present work assigns it as some fraction of the centerline concentration, as it is done for the Gaussian plume equation [18], where 10% of the centerline concentration is considered to be zero. Solutions for different ratios are compared in Chapter III.

The procedure to obtain the collocation matrix, used to integrate in the along wind direction, is presented next. Since orthogonal collocation is applied to the vertical direction with N_z number of collocation

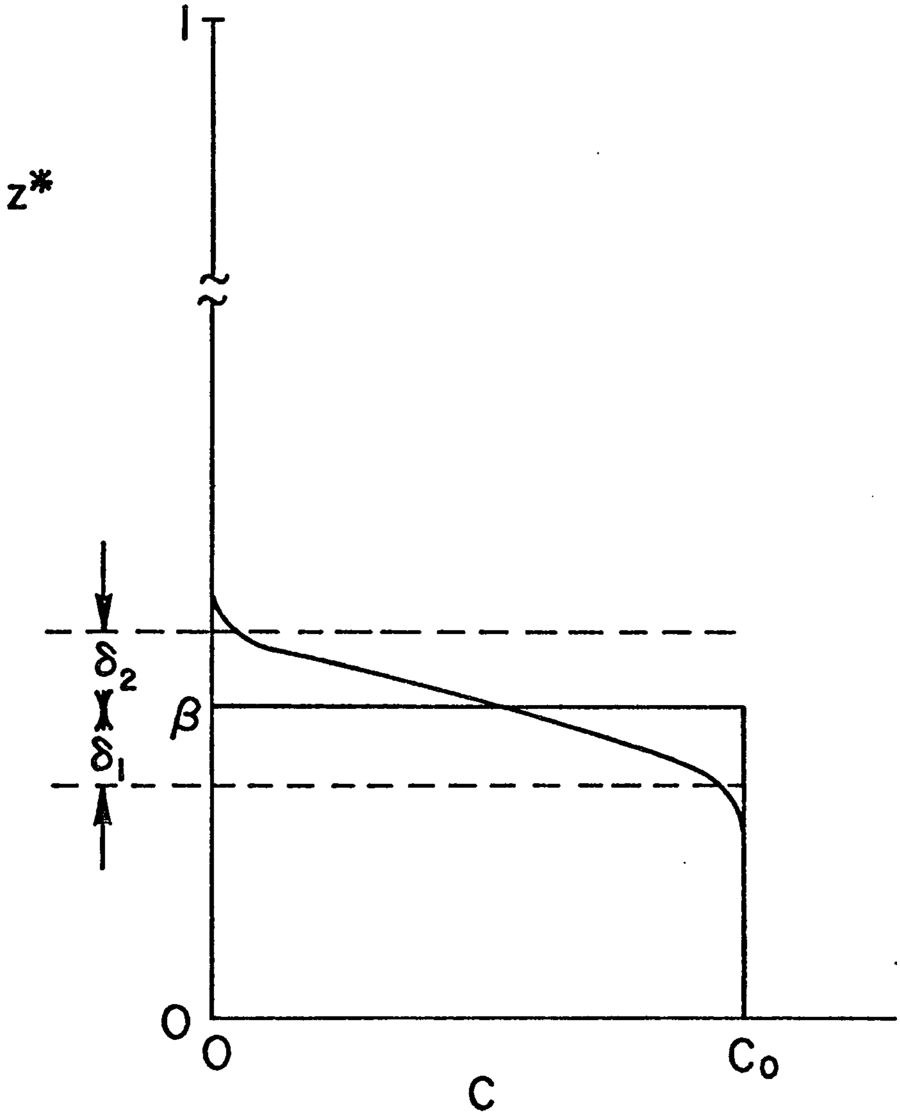

FIGURE 2.2 CORRECT VERTICAL CONCENTRATION DISTRIBUTION AT ANY ξ - GROUND LEVEL LINE SOURCE

points, equation (2.20) remains as

$$R_1 \frac{dC_\ell}{d\xi} = R_5 \sum_{i=1}^{N_z+2} B_{\ell i} C_i \qquad , \text{ for } \ell=2,\ldots,N_z+1 \tag{2.23}$$

The application of orthogonal collocation to the boundary conditions, equation (2.22), gives the following expressions:

$$\begin{aligned} \sum_{i=1}^{N_z+2} A_{1,i} C_i &= 0 \qquad \text{at} \qquad \zeta=0 \\ \sum_{i=1}^{N_z+2} A_{N_z+2,i} C_i &= 0 \qquad \text{at} \qquad \zeta=1 \end{aligned} \tag{2.24}$$

Solving for the concentration at the boundaries C_1 and C_{N_z+2} as functions of the concentrations at the interior collocation points one obtains

$$C_1 = - \frac{\sum_{i=2}^{N_z+1} A1(i) C_i}{A_{1,1}} \tag{2.25}$$

$$C_{N_z+2} = \frac{\sum_{i=2}^{N_z+1} A2(i) C_i}{DEN} \tag{2.26}$$

where

$$A1(i) = A_{1,i} + \frac{A_{1,N_z+2}\, A2(i)}{DEN} \tag{2.27}$$

$$A2(i) = A_{1,1} A_{N_z+2,i} - A_{N_z+2,1} A_{1,i} \tag{2.28}$$

$$DEN = A_{N_z+2,1}A_{1,N_z+2} - A_{1,1}A_{N_z+2,N_z+2} \qquad (2.29)$$

Finally, by substituting equations (2,25) and (2.26), equation (2.23) in matrix notation remains as follows:

$$\frac{d\underline{C}}{d\xi} = \underline{\underline{E}}\,\underline{C} \qquad (2.30)$$

where the elements of the matrix E are

$$E_{\ell i} = -\frac{R_5 B_{\ell,1} A1(i)}{R_1 A_{1,1}} + \frac{R_5 B_{\ell i}}{R_1} + \frac{R_5 B_{\ell,N_z+2} A2(i)}{R_1\ DEN} \qquad (2.31)$$

The solution of equation (2.30) is given by:

$$\underline{C}(\xi) = \underline{\underline{U}}\ \exp\ (\underline{\underline{\Lambda}}\xi)\underline{\underline{U}}^{-1}\underline{C}^{i}(\xi-\Delta\xi) \qquad (2.32)$$

where $\underline{\underline{U}}$, $\underline{\underline{\Lambda}}$, and $\underline{\underline{U}}^{-1}$ are the eigenvectors, eigenvalues (diagonal), and eigenrows of the matrix E, respectively. The diagonalization of the collocation matrix E is performed by a subroutine called EISYS [12] such that $\underline{\underline{U}}$, $\underline{\underline{\Lambda}}$, and $\underline{\underline{U}}^{-1}$ can be obtained. Since the collocation matrix depends on the parameters δ_1 and δ_2, its eigenvalues, eigenvectors and eigenrows have to be recalculated any time δ_1 and/or δ_2 change.

The determination of the initial condition $\underline{C}^{i}$ needed to solve equation (2.30) when $\xi>0$ uses the solution of $\underline{C}$ for the previous integration step $\Delta\xi$. If neither δ_1 nor δ_2 are changed, $\underline{C}^{i}(\xi-\Delta\xi)$ is equated to $\underline{C}(\xi-\Delta\xi)$. When the parameters δ_1 and/or δ_2 change, the initial condition is obtained through a Lagrangian interpolation of the previous good solution and the integration is repeated. This interpolation occurs only for the new position of the collocation points which lie within the previous region $[\beta-\delta_1, \beta+\delta_2]$. For points to the left of $(\beta-\delta_1)$ and to the right of $(\beta+\delta_2)$ values of C_o and zero are assigned to the concentrations, respectively.

The flux at any position in the along wind direction is a useful piece of information that can be obtained from the results and provides a check for continuity. It can be expressed by the following equation:

$$Q_x = \int_o^{z_{max}} u\ C(x,z)dz \tag{2.33}$$

Transformation of the spatial variables gives

$$Q_x = \int_o^1 u\ C(\xi,z^*)z_{max}\ dz^* \tag{2.34}$$

By substituting equation (2.19) one obtains

$$Q_x = \int_o^{\beta-\delta_1} u\ C_o z_{max} d\zeta + \int_{\beta-\delta_1}^{\beta+\delta_2} u\ C(\xi,\zeta)z_{max}\ d\zeta \tag{2.35}$$

Finally, using Gaussian quadrature weights, equation (2.35) can be transformed to

$$Q_x = Q_x^1 + uz_{max}(\delta_1+\delta_2)\sum_{i=1}^{N_z+2} W_i C_i \tag{2.36}$$

where

$$Q_x^1 = \begin{cases} u\ z_{max}(\beta-\delta_1)C_o & \text{for} \quad \delta_1<\beta \\ 0 & \text{for} \quad \delta_1=\beta \end{cases} \tag{2.37}$$

Two Dimensional-Continuous Elevated Line Source

Treatment of the two-dimensional diffusion equation (2.11) for the case of an elevated line source gives more generality to an air pollution model. The only variation with respect to the previous case takes place in the boundary condition (2.7b), which is transformed to:

$$C \to \infty \qquad \text{at} \qquad x = 0 \quad \text{and} \quad z = H \tag{2.38}$$

The analytical solution to this problem is given by

$$C(x,z) = \frac{Q}{2[\pi\, u\, K_z x]^{\frac{1}{2}}} \left(\exp\left(- \frac{u(z-H)^2}{4K_z x}\right) + \exp\left(- \frac{u(z+H)^2}{4K_z x}\right) \right) \tag{2.39}$$

The technique for solving this case is the same as the previous one, but with a different representation of the concentration distribution at x=0, as shown in Figure 2.3. This discontinuous initial value profile is expressed as:

$$C^i = \begin{cases} C_o & \text{at} \quad \xi = 0 \;, \quad h - \beta \le z^* \le h + \beta \\ 0 & \text{at} \quad \xi = 0 \;, \quad \text{elsewhere} \end{cases} \tag{2.40}$$

with

$$h = \frac{H}{z_{max}} \tag{2.41}$$

and

$$C_o = \frac{Q}{2u\beta z_{max}} \tag{2.42}$$

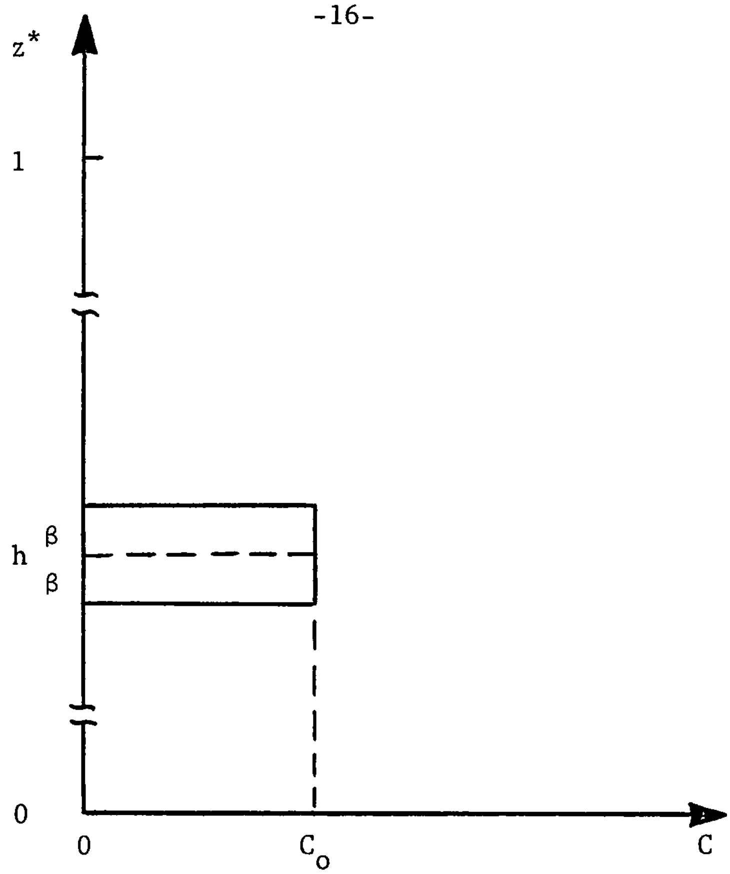

FIGURE 2.3 VERTICAL CONCENTRATION DISTRIBUTION AT x=0 - ELEVATED LINE SOURCE

In order to apply orthogonal collocation to the entire region of interest in the z direction, and taking into account that β is very small compared to 1, the following variable tranformation is performed:

$$z^* = (\delta_1 + \delta_2 + 2\beta)\zeta + h - (\beta + \delta_1) \tag{2.43}$$

where $0 \leq \zeta \leq 1$. The coefficients in equation (2.20) remain then as,

$$R_1 = \frac{u}{x_{max}} \quad ; \quad R_5 = \frac{K_z}{z_{max}^2(\delta_1+\delta_2+2\beta)^2} \tag{2.44}$$

The concentration distribution is now obtained only within the $[h-\beta-\delta_1,\ h+\beta+\delta_2]$ interval in the z* domain, as shown in Figure 2.4.

The check on the parameters δ_1 and δ_2 is done with the same previous criteria, but now the concentrations at $\zeta=0$ and $\zeta=1$ are both compared to zero (= some fraction of the centerline concentration). The comparison at $\zeta=0$ stops when the plume has reached the ground, i.e., $\delta_1=h-\beta$, and stops at $\zeta=1$ when the plume reaches the inversion layer, i.e., $\delta_2=1-(h+\beta)$.

The calculation of the collocation matrix and its diagonalization to obtain the eigenvalues, eigenvectors and eigenrows follows the same procedure as before, with its elements $E_{\ell i}$ given by equation (2.31). The solution to this problem is also determined by equation (2.32).

The initial condition $\underline{C}^i$ at any integration step is calculated in the same way as previously discussed. Whenever an interpolation is needed for this purpose, zero concentration is assigned to every new collocation point that lies outside the region of interest $[h-\beta-\delta_1,\ h+\beta+\delta_2]$ used for the previous step.

Equation (2.34) can be utilized to determine the flux at any position in the x direction. Substitution of equation (2.43) into (2.34) and the use of Gaussian quadrature weights gives the following expression:

$$Q_x = u\ z_{max}(2\beta+\delta_1+\delta_2) \sum_{i=1}^{N_z+2} W_i C_i \tag{2.45}$$

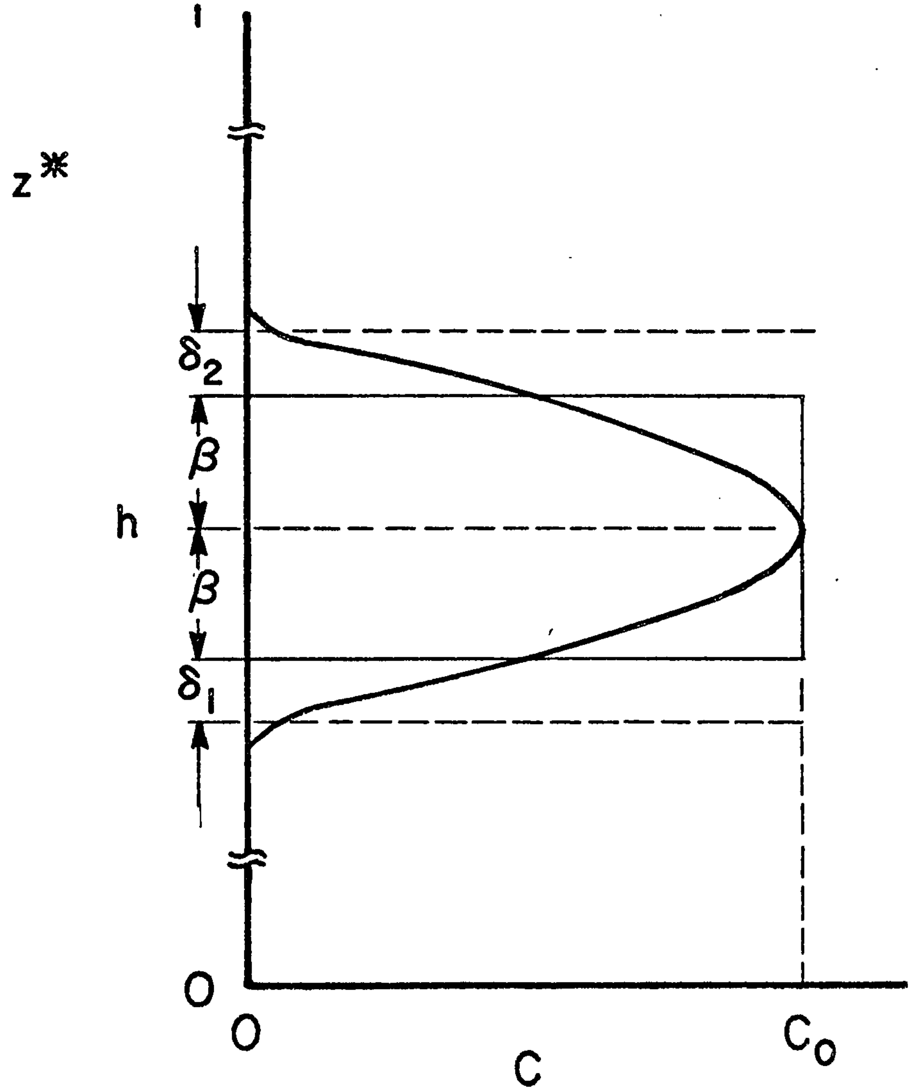

FIGURE 2.4 CORRECT VERTICAL CONCENTRATION DISTRIBUTION AT ANY ξ - ELEVATED LINE SOURCE

Two Dimensional Models with Chemical Reactions

The next step in complexity of an air pollution model is to consider a line source case with a pollutant undergoing some kind of removal process, usually expressed as a chemical reaction. Steady-state models for reactive contaminants do not exist because conditions under which reactive pollutant concentrations are not changing with time are virtually non-existent. In spite of this, a solution to this problem is presented next since few modifications to the previous cases are required and its study will help to understand more complex models like the unsteady-state point source case.

The main difference between this case and the previous models occurs in equation (2.11). An additional term, which represents the chemical reaction, should be incorporated in the diffusion equation as

$$u \frac{\partial C}{\partial x} = K_z \frac{\partial^2 C}{\partial z^2} + R \tag{2.46}$$

The technique for solving the collocation equations that arise from equation (2.11), using the eigenvalues of the collocation matrix, is still valid for equation (2.46) if a first-order reaction model is utilized to represent pollutant removal from the atmosphere:

$$R = -k_1 C \tag{2.47}$$

The elements of the collocation matrix would now be given by

$$E_{\ell i} = - \frac{R_5 B_{\ell,1} A1(i)}{R_1 \; A_{1,1}} + \frac{R_5 B_{\ell i}}{R_1} + \frac{R_5 B_{\ell,N_z+2} A2(i)}{R_1 \; DEN} - \frac{k_1}{R_1} \delta_{\ell i} \tag{2.48}$$

where $\delta_{\ell i}$ is the Knonecker delta function,

$$\delta_{\ell i} = \begin{cases} 1 & \text{for} \quad \ell = i \\ 0 & \text{for} \quad \ell \neq i \end{cases} \tag{2.49}$$

While this is the only modification that should be incorporated in the elevated line source model, two more changes should be considered in the ground line source case.

The check on the parameter δ_1 must be performed with another criteria, i.e., if $\delta_1 < \beta$, the calculated concentration at $\zeta=0$ should be compared to $C_o \exp(-\frac{k_1 x}{u})$. The reason being the disappearance of contaminant due to the chemical reaction.

The other modification takes place in the calculation of the flux at any position in the x-direction. Equation (2.35) remains then as follows:

$$Q_x = \int_o^{\beta-\delta_1} u C_o e^{-\frac{k_1 \xi}{R_1}} z_{max} d\zeta + \int_{\beta-\delta_1}^{\beta+\delta_1} u C(\xi,\zeta) z_{max} d\zeta \tag{2.50}$$

Therefore, equation (2.36) would contain,

$$Q_x^1 = \begin{cases} uz_{max}(\beta-\delta_1)C_o e^{-\frac{k_1\xi}{R_1}} & \text{for} \quad \delta_1<\beta \\ 0 & \text{for} \quad \delta_1=\beta \end{cases} \tag{2.51}$$

The procedure to follow for non-linear chemical reaction models would be to linearize the expression if the eigenvalue method is to be used. Another possibility, simpler and more effective, is to integrate the collocation equations with a technique that would not depend on the expression for the removal processes, e.g., a fourth-order Runge-Kutta method.

The concentration distribution for a continuous ground level line source for a case with a first-order chemical reaction model is presented in Chapter IV.

<u>Three Dimensional-Continuous Point Source</u>

For a source which is continuously releasing material at a fixed point, the appropriate form of equation (2.1) (again with v and w zero, and neglecting the diffusion in the x-direction relative to convection) is

$$u\,\frac{\partial C}{\partial x} = \frac{\partial}{\partial y}\left(K_y\,\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\,\frac{\partial C}{\partial z}\right) + R \tag{2.52}$$

At an early stage, observations of diffusion implied a dependence of K_y on the distance of travel [14]. On the grounds that it is physically irrational to regard K_y as a function of horizontal position, one approach has been to seek solutions with K_y, as well as K_z and u, a function of height above the ground, i.e.,

$$u = u(z) \quad ; \quad K_y = K_y(z) \quad ; \quad K_z = K_z(z) \tag{2.53}$$

For this case, equation (2.52) remains as,

$$u(z)\,\frac{\partial C}{\partial x} - \frac{dK_z(z)}{dz}\,\frac{\partial C}{\partial z} = K_y(z)\,\frac{\partial^2 C}{\partial y^2} + K_z(z)\,\frac{\partial^2 C}{\partial z^2} + R \tag{2.54}$$

Consider an interval $[0, y_{max}]$ as the region of interest in the crosswind direction y, where a concentration distribution is to be obtained. For simplicity, the point source is located at y=0, such that no contaminant flows across the centerline y=0. The reason being symmetry, only the x-component of the wind velocity is taken into account. Therefore, the same approaches previously discussed can be used for this three-dimensional continuous point source model.

The crosswind dimension, a subset of the present case, can be considered as an analog of the two-dimensional continuous ground level line source. In addition, the two-dimensional continuous elevated line source can be used to represent the other subset, i.e., the vertical dimension. The reason for different approaches for each spatial dimension is that the concentration distribution in the crosswind direction is symmetric with respect to the centerline (y=0), whereas the concentration distribution in the vertical direction is not symmetric with respect to the effective emission height (z=H). The solution in the z-direction would be symmetric if K_z and u were constant, and moreover only up to an x-position where the plume reaches the ground or the inversion layer.

Using the spline collocation approach, the following spatial variables transformations must be made:

$$\frac{y}{y_{max}} = y^* = (\delta_{1y} + \delta_{2y})\eta + \beta_y - \delta_{1y} \tag{2.55}$$

$$\frac{z}{z_{max}} = z^* = (\delta_{1z} + \delta_{2z} + 2\beta_z)\zeta + h - (\beta_z + \delta_{1z}) \tag{2.56}$$

where $0 \le \eta \le 1$ and $0 \le \zeta \le 1$, and h is given by equation (2.41).

The dimensionless variable in the x-direction, presented in equation (2.15), is also introduced in the problem.

For completeness of the model, the following boundary conditions are used:

$$C^i = \begin{cases} C_o & \text{at point source, } \xi=0 \text{ ; } y^*=0 \text{ ; } z^*=h \\ 0 & \text{elsewhere, } \xi=0 \end{cases} \tag{2.57}$$

$$\frac{\partial C}{\partial \eta} = 0 \qquad \text{at} \qquad \eta=0,1 \tag{2.58}$$

$$\frac{\partial C}{\partial \zeta} = 0 \qquad \text{at} \qquad \zeta=0,1 \tag{2.59}$$

where the equivalent concentration at the point source can be calculated by continuity, as will be seen later.

This approach can be used to simulate any three-dimensional continuous point source model, eg., few modifications must be done if the point source is located at the ground, i.e., equation (2.56) would be replaced by another equation (2.55) for the vertical direction; any type of removal process for the contaminant, e.g., sedimentation would be valid since equation (2.59) means no flux at $\zeta=0,1$ and not at the effective emission height, h.

The use of spline collocation for this case again means that the solution is obtained with moving boundary conditions in the y and z directions. Since no changes in the technique were needed, as compared to the previous cases, the check and modifications on δ_1 and δ_2 for each direction at any integration step in the x-direction are performed as before.

The collocation equations for two different situations, constant u, K_y, and K_z, and then as functions of elevation are presented next.

Constant Mean Wind Velocity and Turbulent Diffusivities

Substituting equations (2.15), (2.55) and (2.56) into equation (2.54) (with $\frac{dK_z}{dz} = 0$) one obtains

$$R_1 \frac{\partial C}{\partial \xi} = R_5 \frac{\partial^2 C}{\partial \eta^2} + R_6 \frac{\partial^2 C}{\partial \zeta^2} + R(C) \tag{2.60}$$

where

$$R_1 = \frac{u}{x_{max}} \tag{2.61}$$

$$R_5 = \frac{K_y}{y_{max}^2(\delta_{1y}+\delta_{2y})^2} \tag{2.62}$$

$$R_6 = \frac{K_z}{z_{max}^2(\delta_{1z}+\delta_{2z}+2\beta_z)^2} \tag{2.63}$$

Application of orthogonal collocation to equation (2.60), with N_y and N_z as the number of interior collocation points in the y and z directions, respectively, gives

$$R_1 \frac{dC_{k\ell}}{d\xi} = R_5 \sum_{i=1}^{N_y+2} B_{ki}^{(2)} C_{i\ell} + R_6 \sum_{i=1}^{N_z+2} B_{\ell i}^{(3)} C_{ki} + R(C_{k\ell}) \tag{2.64}$$

$$\text{for} \qquad k=1,\ldots,N_y+2$$
$$\ell=1,\ldots,N_z+2$$

where $C_{k\ell}$ represents the mean concentration at the point (η_k,ζ_ℓ). The superscripts of the discretizational matrix of second derivatives B, represent the direction and thus the way it is computed, i.e., (2) and (3) stand for the y and z directions, respectively.

The use of orthogonal collocation to the boundary conditions in the y-direction, equation (2.58) gives the following expressions:

$$\sum_{i=1}^{N_y+2} A_{1,i}^{(2)} C_{i\ell} = 0 \qquad \text{at} \qquad \eta=0$$

$$\sum_{i=1}^{N_y+2} A_{N_y+2,i}^{(2)} C_{i\ell} = 0 \qquad \text{at} \qquad \eta=1 \tag{2.65}$$

Solving for the concentration at the centerline and at the edge of the plume one obtains,

$$C_{1,\ell} = - \frac{\sum_{i=2}^{N_y+1} A1Y(i) C_{i\ell}}{A^{(2)}_{1,1}} \tag{2.66}$$

$$C_{N_y+2,\ell} = \frac{\sum_{i=2}^{N_y+1} A2Y(i) C_{i\ell}}{DENY} \tag{2.67}$$

where

$$A1Y(i) = A^{(2)}_{1,i} + \frac{A^{(2)}_{1,N_y+2}\ A2Y(i)}{DENY} \tag{2.68}$$

$$A2Y(i) = A^{(2)}_{1,1} A^{(2)}_{N_y+2,i} - A^{(2)}_{N_y+2,1}\ A^{(2)}_{1,i} \tag{2.69}$$

$$DENY = A^{(2)}_{N_y+2,1}\ A^{(2)}_{1,N_y+2} - A^{(2)}_{1,1}\ A^{(2)}_{N_y+2,N_y+2} \tag{2.70}$$

Application of orthogonal collocation to the boundary conditions in the z-direction, equation (2.59) gives:

$$\begin{aligned} \sum_{i=1}^{N_z+2} A^{(3)}_{1,i}\ C_{ki} &= 0 \qquad \text{at} \qquad \zeta=0 \\ \sum_{i=1}^{N_z+2} A^{(3)}_{N_z+2,i}\ C_{ki} &= 0 \qquad \text{at} \qquad \zeta=1 \end{aligned} \tag{2.71}$$

Following the same procedure as for the y-direction, the concentration at the edges of the plume in the z-domain is obtained from equation (2.71):

$$C_{k,1} = - \frac{\sum_{i=2}^{N_z+1} A1Z(i) C_{ki}}{A^{(3)}_{1,1}} \tag{2.72}$$

$$C_{k,N_z+2} = \frac{\sum_{i=2}^{N_z+1} A2Z(i) C_{ki}}{DENZ} \tag{2.73}$$

where

$$A1Z(i) = A^{(3)}_{1,i} + \frac{A^{(3)}_{1,N_z+2} \; A2Z(i)}{DENZ} \tag{2.74}$$

$$A2Z(i) = A^{(3)}_{1,1} A^{(3)}_{N_z+2,i} - A^{(3)}_{N_z+2,1} A^{(3)}_{1,i} \tag{2.75}$$

$$DENZ = A^{(3)}_{N_z+2,1} A^{(3)}_{1,N_z+2} - A^{(3)}_{1,1} A^{(3)}_{N_z+2,N_z+2} \tag{2.76}$$

Substituting equations (2.66), (2.67), (2.72), and (2.73) into equation (2.64) one obtains,

$$R_1 \frac{dC_{k\ell}}{d\xi} = R_5 \left(\sum_{i=2}^{N_y+1} \left(- B^{(2)}_{k,1} \frac{A1Y(i)}{A^{(2)}_{1,1}} + B^{(2)}_{ki} + B^{(2)}_{k,N_y+2} \frac{A2Y(i)}{DENY}\right) C_{i\ell} \right) +$$

$$R_6 \left(\sum_{i=2}^{N_z+1} \left(- B^{(3)}_{\ell,1} \frac{A1Z(i)}{A^{(3)}_{1,1}} + B^{(3)}_{\ell i} + B^{(3)}_{\ell,N_z+2} \frac{A2Z(i)}{DENZ}\right) C_{ki} \right)$$

$$+ R(C_{k\ell}) \tag{2.77}$$

or simplifying it:

$$\frac{dC_{k\ell}}{d\xi} = \frac{R_5}{R_1} \left(\sum_{i=2}^{N_y+1} AKY(k,i) C_{i\ell} \right) + \frac{R_6}{R_1} \left(\sum_{i=2}^{N_z+1} AKZ(\ell,i) C_{ki} \right) +$$

$$+ \frac{R(C_{k\ell})}{R_1} \tag{2.78}$$

for $k=2,\ldots,N_y+1$

$\ell=2,\ldots,N_z+1$

Equation (2.78) gives a set of $(N_y)(N_z)$ first-order ordinary differential equations to solve for the concentration as a function of the along wind direction at the orthogonal collocation points in the crosswind and vertical directions. The initial condition for this system of equations is

$$C^i_{k\ell} = \begin{cases} C_o & \text{at} \quad \xi=0 \,, \quad 0 \le y^* \le \beta_y \\ & \qquad\qquad h - \beta_z \le z^* \le h + \beta_z \\ 0 & \text{at} \quad \xi=0 \,, \quad y^* > \beta_y \\ & \qquad\qquad \text{elsewhere } z^* \end{cases} \tag{2.79}$$

Using continuity, the flux at the point source can be expressed as:

$$Q = 2 \int_o^{\beta_y} \int_{-\beta_z}^{\beta_z} u(h) C_o y_{max} dy^* z_{max} dz^* \tag{2.80}$$

Solving for C_o, the equivalent concentration at the source one obtains,

$$C_o = \frac{Q}{4u(h)\beta_z z_{max} \beta_y y_{max}} \tag{2.81}$$

For a ground level point source, the 4 in the denominator should be replaced by a 2.

The determination of the initial condition at any integration step follows the same procedure as before. If the concentration at the edges of the plume lies within the range specified by a fraction of the centerline concentration, the solution of the current step is used as the initial condition for the next step. For any boundary concentration outside this comparison, the corresponding δ parameter must be changed. If this occurs, the new positions of the collocation points have to be calculated by equations (2.55) and/or (2.56) and the concentration at these points determined through Lagrangian interpolation in two dimensions using the good solution of the previous step. This will be then the initial condition used at the current integration step. For simplicity, δ_{1y} is equated to β_y such that the comparisons are performed strictly to the boundary concentrations at $\eta=1$, $\zeta=0$ and $\zeta=1$.

In order to apply the technique to any air pollution model, i.e., with any type of removal processes, the eigenvalue method for obtaining the solution was dropped. This method has the attractive feature that whenever the region of interest does not change, the same eigenvalues, eigenvectors and eigenrows for the previous step can be used for the current step. That is, the rediagonalization of the collocation matrix must not be done at every integration step, which results in computational time savings. But in view of generality, other integration techniques were investigated.

A semi-implicit Runge-Kutta technique, based on the method proposed by Caillaud and Padmanabhan [3] was developed in the present work. This type of technique is applied to difficult stiff differential equations. As soon as the stiff component has faded away, at certain position from the point source, it becomes desirable to enlarge the stepsize. A stepsize adjustment algorithm, proposed by Villadsen [19] was used in the present work. This integration method appeared to be very stable and the calculated concentration distribution was the same as that determined by the eigenvalue technique. Unfortunately, the complexity of the present air pollution model requires a large number of differential equations to be solved. The use of both methods involved a large computational time.

Finally DRKGS, a double precision subroutine furnished by IBM [11] which is a fourth-order Runge-Kutta method, was applied to the present problem. The use of this subroutine was discussed in details by Fleischer [8]. It was decided to keep it as the integration method for all three-dimensional models since the results were comparable to the ones obtained using the previous two methods, but with less than half of their computational time.

The present work for the case of no chemical reactions was validated by comparing the results to the Gaussian plume equation given by

$$C(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z u} \exp\left(-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right)\left(\exp\left(-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right)\right) \tag{2.82}$$

and to the analytical solution of the diffusion equation with a reflecting plane at the ground z=0, given by

$$C(x,y,z) = \frac{Q}{4\pi x(K_yK_z)^{\frac{1}{2}}} \exp\left(-\frac{uy^2}{4K_yx}\right)\left(\exp\left(-\frac{u(z-H)^2}{4K_zx}\right) + \exp\left(-\frac{u(z+H)^2}{4K_zx}\right)\right) \tag{2.83}$$

The flux across any plane normal to the x axis is also calculated in the present work via

$$Q_x = 2\int_o^{y_{max}}\int_o^{z_{max}} u\ C(x,y,z)dydz \qquad (2.84)$$

Substituting equations (2.55) and (2.56), and using Gaussian quadrature weights, equation (2.84) can be transformed to

$$Q_x = 2u(\delta_{1y}+\delta_{2y})y_{max}(\delta_{1z}+\delta_{2z}+2\beta_z)z_{max}\sum_{k=1}^{N_y+2}\sum_{\ell=1}^{N_z+2} W_k^{(2)}W_\ell^{(3)}C_{k\ell} \qquad (2.85)$$

Variable Mean Wind Velocity and Turbulent Diffusivities

The governing equation for this case, equation (2.54), with the incorporation of the spatial variable transformations given by equations (2.15), (2.55) and (2.56) can be expressed as follows:

$$R_1(\zeta)\frac{\partial C}{\partial \xi} + R_3(\zeta)\frac{\partial C}{\partial \zeta} = R_5(\zeta)\frac{\partial^2 C}{\partial \eta^2} + R_6(\zeta)\frac{\partial^2 C}{\partial \zeta^2} + R(C) \qquad (2.86)$$

where

$$R_1(\zeta) = \frac{u(\zeta)}{x_{max}} \qquad (2.87)$$

$$R_3(\zeta) = -\frac{\frac{dK_z}{dz}(\zeta)}{z_{max}(\delta_{1z}+\delta_{2z}+2\beta_z)} \qquad (2.88)$$

$$R_5(\zeta) = \frac{K_y(\zeta)}{y_{max}^2(\delta_{1y}+\delta_{2y})^2} \tag{2.89}$$

$$R_6(\zeta) = \frac{K_z(\zeta)}{z_{max}^2(\delta_{1z}+\delta_{2z}+2\beta_z)^2} \tag{2.90}$$

The procedure to obtain the collocation equations is exactly the same as the one previously done, with one extra term involving $R_3(\zeta)\,\frac{\partial C}{\partial \zeta}$ in these equations. The final expression then is given by

$$\frac{dC_{k\ell}}{d\xi} = -\frac{R_3(\ell)}{R_1(\ell)}\left(\sum_{i=2}^{N_z+1} \mathrm{DAKZ}(\ell,i)C_{ki}\right) + \frac{R_5(\ell)}{R_1(\ell)}\left(\sum_{i=2}^{N_y+1} \mathrm{AKY}(k,i)C_{i\ell}\right) +$$

$$\frac{R_6(\ell)}{R_1(\ell)}\left(\sum_{i=2}^{N_z+1} \mathrm{AKZ}(\ell,i)C_{ki}\right) + \frac{R(C_{k\ell})}{R_1(\ell)} \tag{2.91}$$

for $k=2,\ldots,N_y+1$

$\ell=2,\ldots,N_z+1$

where

$$\mathrm{DAKZ}(\ell,i) = -A_{\ell,1}^{(3)}\,\frac{\mathrm{A1Z}(i)}{A_{1,1}^{(3)}} + A_{\ell i}^{(3)} + A_{\ell,N_z+2}^{(3)}\,\frac{\mathrm{A2Z}(i)}{\mathrm{DENZ}} \tag{2.92}$$

and AKY(k,i), AKZ(ℓ,i), A1Z(i), A2Z(i), and DENZ are the same as before.

The flux across any plane normal to the along wind direction is calculated by an equation similar to (2.85), i.e.,

$$Q_x = 2(\delta_{iy}+\delta_{2y})y_{max}(\delta_{1z}+\delta_{2z}+2\beta_z)z_{max} \sum_{k=1}^{N_y+2} \sum_{\ell=1}^{N_z+2} u(\ell)W_k^{(2)}W_\ell^{(3)}C_{k\ell} \qquad (2.93)$$

Analytical solutions for arbitrary source heights and unrestricted functions of u, K_y and K_z with elevation have not yet been obtained. It should be pointed out that the present technique can be applied to any function of u, K_y and K_z with respect to any spatial variable and meteorological parameter, as will be seen later. Few modifications must be done to the present model for cases involving functional relationship with respect to other spatial variables, besides elevation.

Three Dimensional Mean Wind Velocity

Let us now consider a continuous point source emitting contaminants to a region where the axial and lateral components of the mean wind velocity are important. For this case, equation (2.1) is reduced to:

$$u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \frac{\partial}{\partial y}\left(K_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) + R \qquad (2.94)$$

where the diffusion in the x-direction is again neglected compared to convection, and w is assumed to be zero. Using the same previous functional relationships for the velocities and diffusivities, i.e.,

$$u=u(z); \quad v=v(z); \quad K_y=K_y(z); \quad K_z=K_z(z) \qquad (2.95)$$

equation (2.94) remains as

$$u(z)\frac{\partial C}{\partial x} + v(z)\frac{\partial C}{\partial y} - \frac{dK_z(z)}{dz}\frac{\partial C}{\partial z} = K_y(z)\frac{\partial^2 C}{\partial y^2} + K_z(z)\frac{\partial^2 C}{\partial z^2} + R \qquad (2.96)$$

The previous approach used for the y-direction is not valid for the present model since the concentration distribution in this dimension is no longer symmetric with respect to the centerline (y=0). For an interval $[-y_{max}, y_{max}]$ as the region of interest in the y-direction, the following variable transformations are performed:

$$y^* = \frac{\frac{y}{y_{max}} + 1}{2} \tag{2.97}$$

$$z^* = \frac{z}{z_{max}} \tag{2.98}$$

$$y^* = (\delta_{1y}+\delta_{2y}+2\beta_y)\eta + \frac{1}{2} - (\beta_y+\delta_{1y}) \tag{2.99}$$

$$z^* = (\delta_{1z}+\delta_{2z}+2\beta_z)\zeta + h - (\beta_z+\delta_{1z}) \tag{2.100}$$

where $0 \leq \eta \leq 1$, $0 \leq \zeta \leq 1$.

The initial condition for this case can then be stated as

$$C^i = \begin{cases} C_o & \text{at point source, } \xi=0;\ y=0(y^*=\tfrac{1}{2});\ z^*=h \\ 0 & \text{elsewhere, } \xi=0 \end{cases} \tag{2.101}$$

Substituting equations (2.97) through (2.100) and equation (2.15) into equation (2.96) one obtains

$$R_1(\zeta)\frac{\partial C}{\partial \xi} + R_2(\zeta)\frac{\partial C}{\partial \eta} + R_3(\zeta)\frac{\partial C}{\partial \zeta} = R_5(\zeta)\frac{\partial^2 C}{\partial \eta^2} + R_6(\zeta)\frac{\partial^2 C}{\partial \zeta^2} + R(C) \tag{2.102}$$

where $$R_1(\zeta) = \frac{u(\zeta)}{x_{max}} \tag{2.103}$$

$$R_2(\zeta) = \frac{v(\zeta)}{2y_{max}(\delta_{1y}+\delta_{2y}+2\beta_y)} \tag{2.104}$$

$$R_3(\zeta) = -\frac{\frac{dK_z}{dz}(\zeta)}{z_{max}(\delta_{1z}+\delta_{2z}+2\beta_z)} \tag{2.105}$$

$$R_5(\zeta) = \frac{K_y(\zeta)}{4y^2_{max}(\delta_{1y}+\delta_{2y}+2\beta_y)^2} \tag{2.106}$$

$$R_6(\zeta) = \frac{K_z(\zeta)}{z^2_{max}(\delta_{1z}+\delta_{2z}+2\beta_z)^2} \tag{2.107}$$

The boundary conditions in the y and z-directions are the same as before, given by equations (2.58) and (2.59). Therefore, application of orthogonal collocation to this model adds only one extra term to the right hand side of equation (2.91):

$$-\frac{R_2(\ell)}{R_1(\ell)}\left(\sum_{i=2}^{N_y+1} AVY(k,i)C_{i\ell}\right) \tag{2.108}$$

with

$$AVY(k,i) = -A^{(2)}_{k,1}\frac{A1Y(i)}{A^{(2)}_{1,1}} + A^{(2)}_{ki} + A^{(2)}_{k,N_y+2}\frac{A2Y(i)}{DENY} \tag{2.109}$$

The initial condition for this system of first-order ordinary differential equations, equation (2.101), can be expressed as,

$$C^i_{k\ell} = \begin{cases} C_o & \text{at} \quad \xi=0, \quad \frac{1}{2} - \beta_y \le y^* \le \frac{1}{2} + \beta_y \\ & \qquad\qquad\;\; h - \beta_z \le z^* \le h + \beta_z \\ 0 & \text{at} \quad \xi=0, \quad \text{elsewhere } y^* \text{ and } z^* \end{cases} \tag{2.110}$$

The equivalent source concentration can again be obtained using continuity:

$$Q = \int_{-\beta_y}^{\beta_y} \int_{-\beta_z}^{\beta_z} u(h) C_o (2y_{max} dy^*) z_{max} dz^* \tag{2.111}$$

Solving for C_o, one obtains

$$C_o = \frac{Q}{8u(h) y_{max} \beta_y z_{max} \beta_z} \tag{2.112}$$

Finally, the flux at any position in the along wind direction can be calculated by

$$Q_x = \int_{-y_{max}}^{y_{max}} \int_{o}^{z_{max}} u(z) C(x,y,z) dy dz \tag{2.113}$$

Using the same procedure as before, equation (2.113) can be reduced to:

$$Q_x = 2(\delta_{1y}+\delta_{2y}+2\beta_y) y_{max} (\delta_{1z}+\delta_{2z}+2\beta_z) z_{max} \sum_{k=1}^{N_y+2} \sum_{\ell=1}^{N_z+2} u(\ell) W_k^{(2)} W_\ell^{(3)} C_{k\ell} \tag{2.114}$$

It should be pointed out that the incorporation of the third component of the mean wind velocity, w(z), into the diffusion equation (2.94) modifies only one term. Equation (2.105) would have to be replaced by the following expression:

$$R_3(\zeta) = \frac{w(\zeta) - \frac{dK_z}{dz}(\zeta)}{z_{max}(\delta_{1z}+\delta_{2z}+2\beta_z)} \qquad (2.115)$$

The procedure to find the edge of the plume in the lateral direction at any integration step is also modified with respect to the previous models. The centerline will not be at y=0, i.e., it might be to the right or left depending upon the direction of the horizontal mean wind velocity.

The concentration at the edges in the y-direction and at the effective emission height, i.e., $C(\eta=0,\ z^*=h)$ and $C(\eta=1,\ z^*=h)$ are compared to a positive or negative value. A negative concentration means that the plume, at that downwind position, is wider than the actual plume, and therefore the parameter δ_{1y} or δ_{2y} is decreased until a positive concentration, at the same x position, is obtained. On the other hand, the same procedure used for the previous models is applied to positive concentrations at the crosswind direction boundaries. Both concentration values are compared to the centerline concentration multiplied by some ratio r, and if they/it are/is larger, the parameter(s) δ_{1y} and/or δ_{2y} are/is increased until the desired accuracy is reached.

CHAPTER III

PARAMETERS ESTIMATION

Basic parameters are estimated for the simple models through parametric studies involving comparison of accuracy and computer time. As the complexity of the models increases, most of these parameters are kept, and others which are inherent of the model in question are estimated for the first time.

Accuracy tests are performed by comparing the calculated concentration values to the analytical solution. For this purpose, an error, which is used throughout this chapter is defined as,

$$e = \left(\frac{C_a - C_c}{C_a}\right)100 \qquad (\%) \qquad (3.1)$$

where the subscripts a and c stand for analytical and calculated, respectively.

The calculations for the present work were done in a UNIVAC 1108 digital computer.

Mathematical Parameters

Two Dimensional-Continuous Ground Level Line Source

The first basic parameter which is estimated is the number of orthogonal collocation points that should be used in calculating the concentration distribution. This parametric study is shown in Figure 3.1. For this case, arbitrary values were assigned to the other

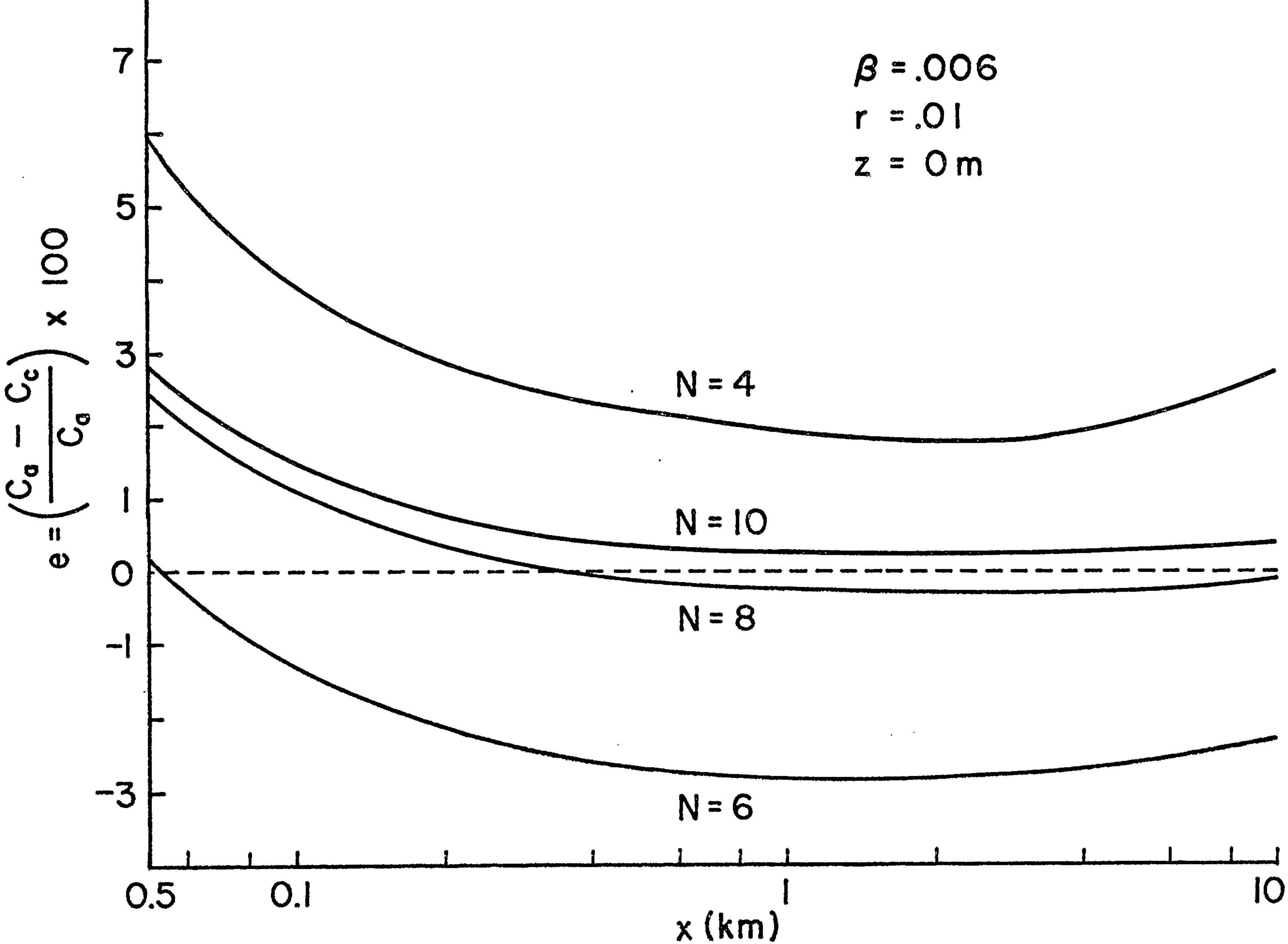

FIGURE 3.1 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON N

parameters remaining, i.e., β was equated to some small value .006, and the ratio of the concentration at the edge of the plume and the centerline concentration was assigned a value of 1%, i.e., r = .01.

Concentration comparisons were performed for the effective emission height, z=0. The other key variable used to select the most convenient number of collocation points, the computer time requirement is shown for each case in Table 3.1.

Table 3.1 Computer Time Requirements for Parametric Study on N - Ground Level Line Source Model

N	Time (sec)
4	7
6	17
8	26
10	46

As it was expected, as N increases the error decreases and the computer time increases. The differences in the computer time spent are not very large with the exception of the last two cases, N=8 and N=10. In addition, the error is greatly minimized as N increases from 4 to 8 interior points, but the difference between the last two cases is negligible. Therefore, the number of interior orthogonal collocation points selected is 8.

The next parametric study done, on β, is shown in Figure 3.2. For this case, r was again given an arbitrary value of 0.01. Time requirements are given in Table 3.2.

Table 3.2 Computer Time Requirements for Parametric Study on β - Ground Level Line Source Model

β	Time (sec)
.003	31
.006	26
.018	32

An analysis for this case shows that as β increases, the error increases for downwind distances close to the emission source. This is exactly one of the objectives pursued in using spline collocation in problems with a discontinuous initial value profile. Since the parameters δ will have a comparable value to β, small values mean that the concentration distribution is calculated only in a region where material exists, i.e., within the plume. This region of interest is very small close to the emission source. As the pollutant moves downwind the plume spreads, and therefore the region of interest is increased by means of the parameters δ.

The computer time requirements for all cases was almost identical, so that a value of .005 was selected for β. Together with the estimation of β, the parameters δ_1 and δ_2 must be specified. The procedure is to

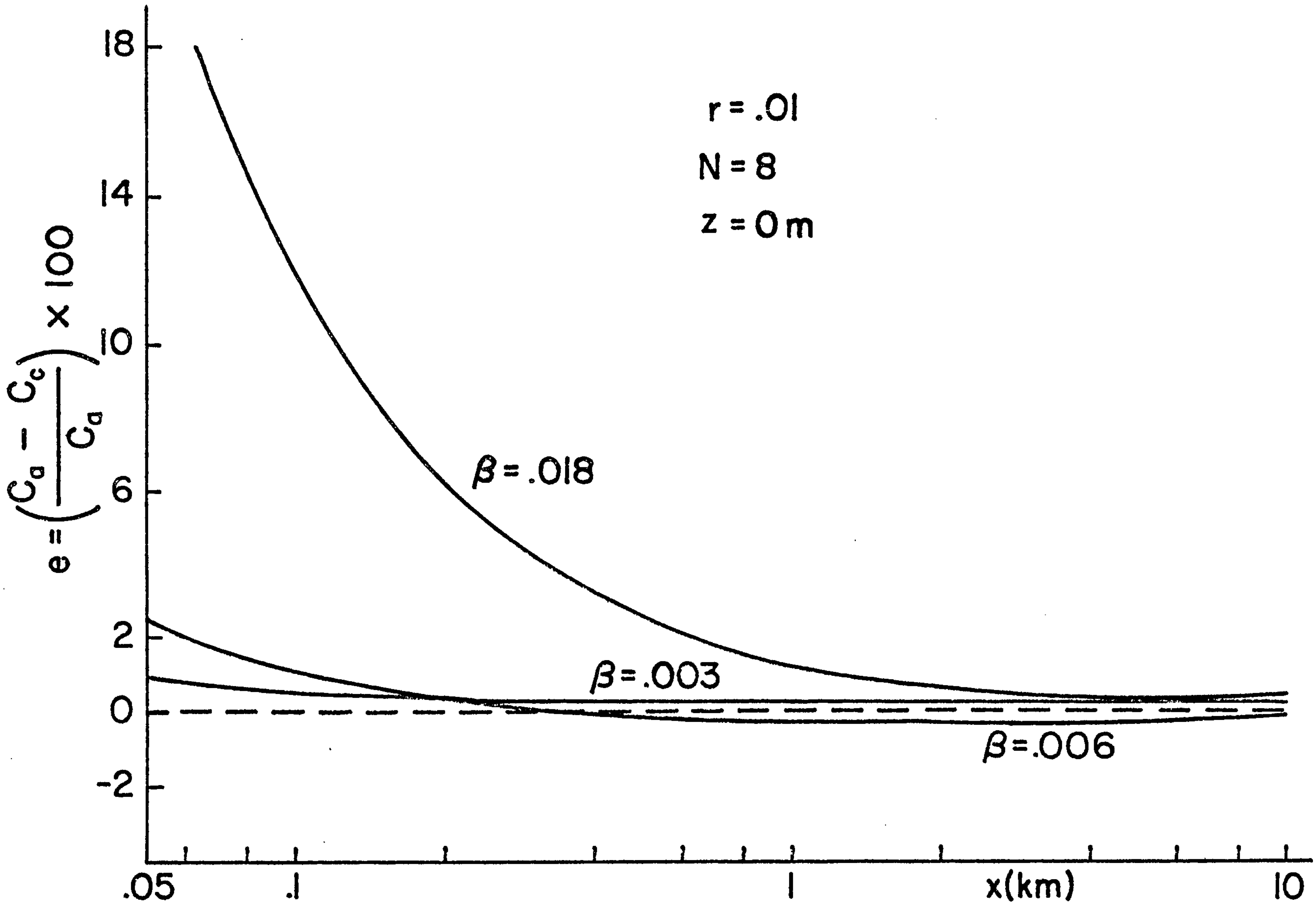

FIGURE 3.2 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON β

find the pair that will determine a region in space which will contain all the material emitted. Since β is very small compared to 1 which is the entire z* domain, the same value of 0.005 was selected for δ_1. In order to estimate δ_2, two cases were simulated in the computer. The first case had a mass flux at the first integration step higher than the emission rate. The other case had Q_x smaller than Q such that a linear interpolation on both δ_2 gave the mass flux equal to the emission rate. The values for an emission rate of 1 gm/m s are shown in Table 3.3.

Table 3.3 Mass Flux vs δ_2 at the First Integration Step - Ground Level Line Source Model

δ_2	Q_x(gm/m s)
.004	.9
.006	1.1
.005	1.0

Everytime the concentration at the boundary is larger than zero, the region of interest is increased by adding .005 to the previous value for δ_2. This "zero concentration" is assigned a certain fraction of the centerline concentration, as it is done in the Gaussian plume equation, where r = .10 (10%). This is then the last basic parameter to be determined for this model, and the results of the parametric study are shown in Figure 3.3 and Table 3.4.

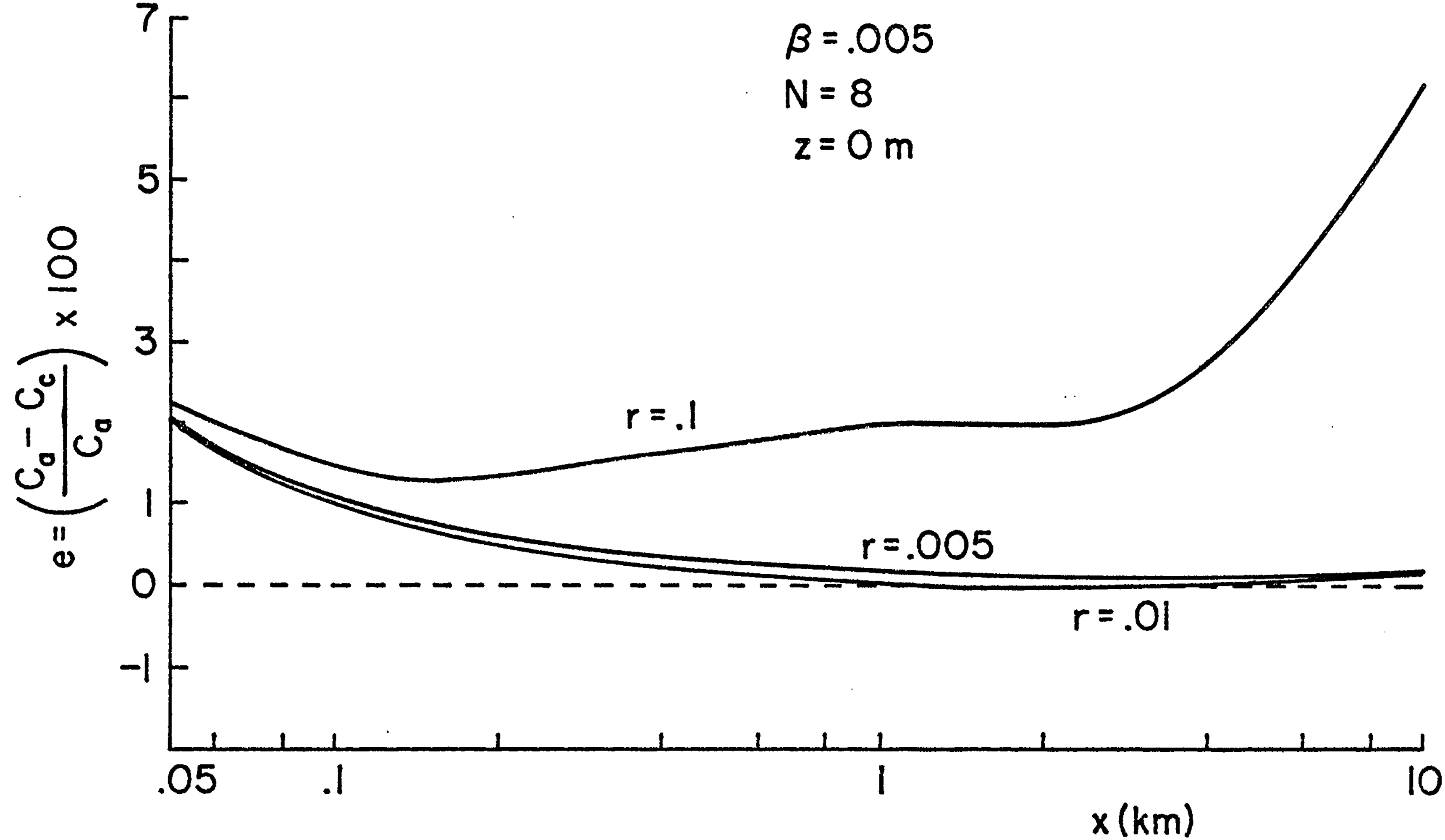

FIGURE 3.3 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON r

Table 3.4 Computer Time requirements for Parametric Study on r - Ground Level Line Source Model

r	Time (sec)
.005	31
.01	27
.1	20

As expected, the lower r the better is the description of the process, i.e., the boundary concentration is closer to zero. But there must be also a compromise in the computer time involved. Therefore, r is assigned a value of 0.01 for the rest of the present work.

There is one more variable in this model that should be analyzed, z_{max}, the maximum elevation. If there is an inversion layer, z_{max} must take on that value. On the other hand, if no inversion layer exists, any value for z_{max} can be specified as input data as long as it does not create an artificial inversion layer. This could happen if x_{max} is very large, e.g., 10 km, and z_{max} very small, e.g., 50 m, such that the plume reaches the maximum elevation before x_{max}.

An increase in the maximum elevation produces a similar effect as increasing β. The region of interest becomes wider such that the accuracy for downwind distances close to the emission source is aggravated. However, every time the parameter δ_2 is increased, a larger z_{max} implies more separation from the ground. This results in fewer situations where the boundary concentration is larger than zero, and thus fewer number of computations. In addition, the separations between interior collocation points in the z domain are larger so that the concentration gradients become smaller. Therefore, the computer time involved is reduced. This analysis is shown in Figure 3.4 and Table 3.5

Table 3.5 Computer Time Requirements for Parametric Study on z_{max} - Ground Level Line Source Model

z_{max}(m)	Time (sec)
50	45
250	40
500	27
1000	16

Figure 3.4 shows incomplete curves for the cases with z_{max} equal to 50 and 250 m. The reason being that at the corresponding downwind position the plume reached the maximum elevation and a comparison to the analytical solution is no longer valid.

The procedure to find the most convenient maximum elevation would be to simulate first a case with a large value for z_{max}, and then by inspecting the results locate the maximum elevation the plume reaches. A value a little bit higher to the one obtained should be assigned to

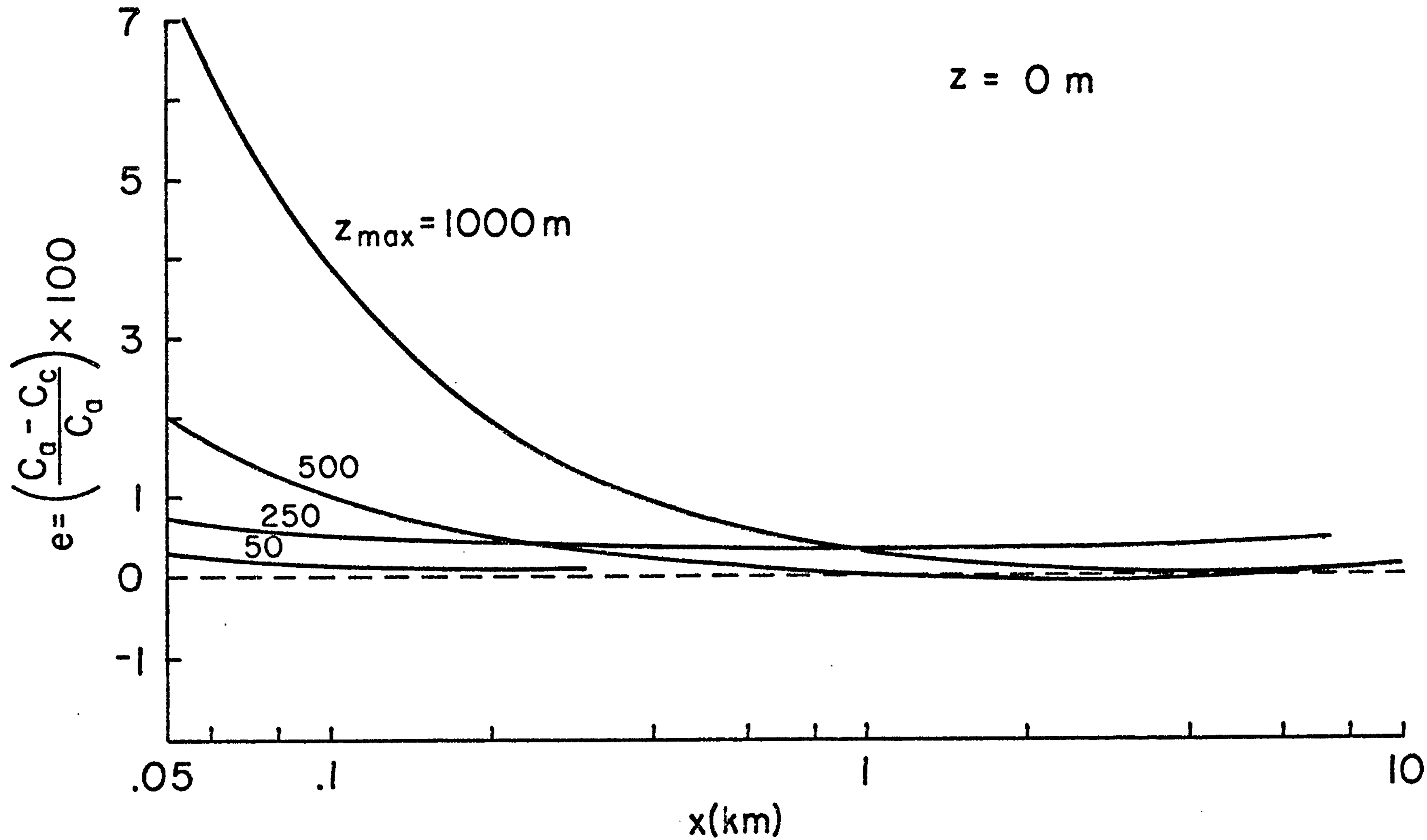

FIGURE 3.4 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON z_{max}

z_{max} if accuracy is the objective. For most cases, z_{max} = 500 m is reasonable enough, unless the problem involves a very unstable atmosphere and/or a very tall stack.

<u>Two Dimensional - Continuous Elevated Line Source</u>

The structure of the technique used to solve this model is different to the previous one in the sense that the parameter β is located to both sides of the effective emission height. For this reason the number of orthogonal collocation points is increased to N = 10.

There is no relation on β for this case and the ground level line source model, so that a parametric study was performed. This is shown in Figure 3.5 and Table 3.6.

Table 3.6 Computer Time Requirements for Parametric Study on β - Elevated Line Source Model

β	Time (sec)
.0010	84
.0012	83
.0013	83
.0014	92
.0015	98
.0020	100

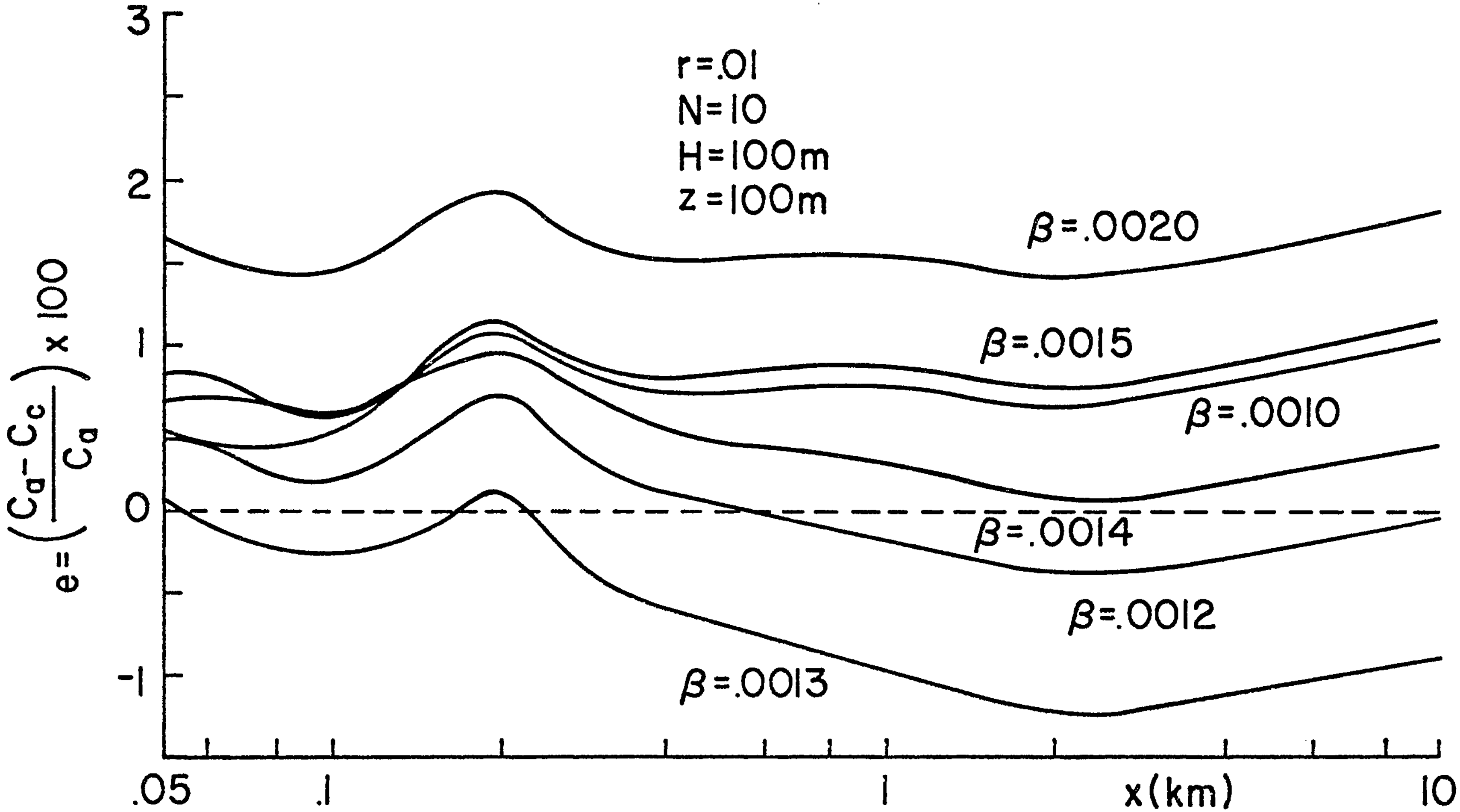

FIGURE 3.5 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT THE EFFECTIVE EMISSION HEIGHT WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON β

The computer time requirements were similar for all cases, so that the selection for β was made on grounds of accuracy. Something very peculiar happens for this approach in the sense that the errors oscillate between zero for the cases of β between .0010 and .0014. No explanation can be given to this, although it is a fact that as β is increased from .0014, the accuracy becomes worse, as it should be and was previously discussed. The errors were computed at the effective emission height, 100 m. It should be pointed out that it would be fortuitous if one of the interior collocation points coincided with the effective emission height. This is the reason why a one-dimensional Lagrangian interpolation was used to obtain the concentration at this elevation. This type of interpolation takes into account the concentration at all collocation points, so that the error calculated at H, besides Q_x, shows the overall error involved in the solution technique.

A value of 0.0012 was assigned for β in this model. The same procedure as before was used to estimate the parameters δ_1 and δ_2. For an emission rate of 1 gm/s m, Table 3.7 shows the final values for δ_1 and δ_2 obtained.

Table 3.7 Mass Flux vs δ_1 and δ_2 at the First Integration Step - Elevated Line Source Model

δ_1	δ_2	Q_x (gm/s)
.0030	.0030	1.0343
.0026	.0026	.9358
.002861	.002861	1.0001

The value by which these parameters are increased whenever the region of interest must be increased is given a similar value as δ_1, i.e., .0025.

The same analysis for z_{max} as previously discussed is presented in Figure 3.6 and Table 3.8. The conclusions are exactly the same, but since the main objective of the present work is accuracy, z_{max} = 500 m is used when possible throughout the entire research.

Table 3.8 Computer Time Requirements for Parametric Study on z_{max} - Elevated Line Source Model

z_{max}(m)	Time (sec)
500	83
2000	27

Three Dimensional Continuous Point Source

Estimation of parameters for this complex model proves that the analysis and understanding of the previous simple cases is valuable. Determination of a convenient set of parameters to get high accuracy would have been difficult without knowledge of the values specified for the previous models.

Let us first consider the case where only one component of the mean wind velocity is taken into account. In addition to u, both turbulent diffusivities, K_y and K_z, are assumed constant.

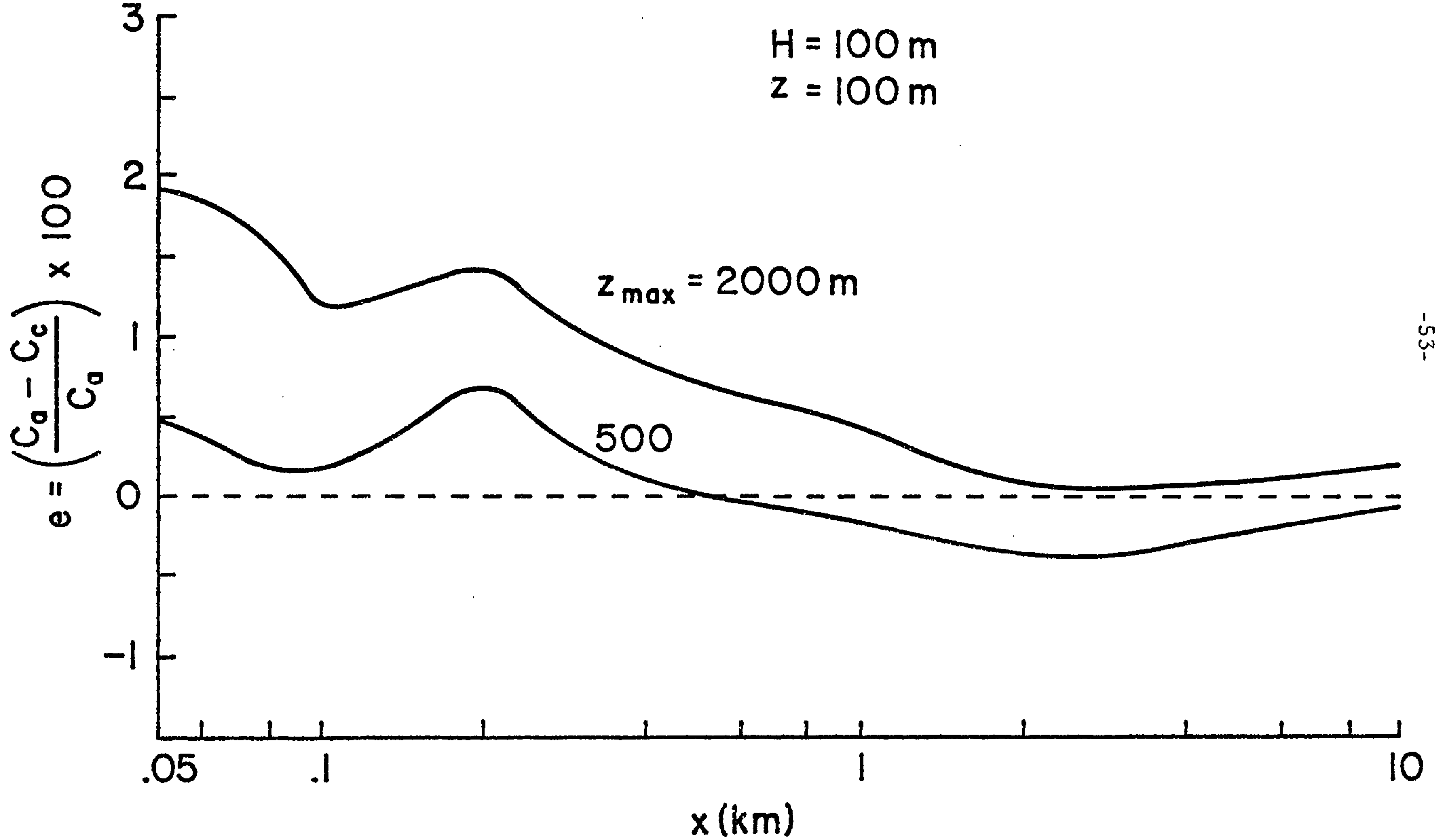

FIGURE 3.6 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT THE EFFECTIVE EMISSION HEIGHT WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON z_{max}

Since the problem can be considered symmetric with respect to the centerline (y=0), the technique utilized for the ground level line source can be used in the lateral direction. Therefore, N_y is equated to 8 and β_y to .005.

In many cases air pollution is due to elevated point sources, so that the approach used for the elevated line source model can be utilized for the z-direction. Therefore, ten interior orthogonal collocation points are used in the vertical dimension, i.e., $N_z = 10$, and a value of 0.0012 is assigned to β_z.

The procedure to obtain the δ parameters, now there are four, follows the one previously discussed. Three of these parameters were given the same value as before, i.e., $\delta_{1y}=.005$, $\delta_{1z}=\delta_{2z}=.002861$ and the fourth parameter was obtained by comparing the mass flux at the first integration step with the emission rate. For this model, Q=1 kg/s, and the parametric study is shown in Table 3.9. A value of .01069 was assigned to δ_{2y}.

Table 3.9 Mass Flux vs δ_{2y} at the First Integration Step - Elevated Point Source Model

δ_{2y}	Q_x(kg/s)
.01	.95607
.011	1.01981
.01069	1.00005

The increments on these parameters, whenever the boundaries of the plume are changed, are the same as the ones used before with the exception of δ_{2y} which now was changed. Again a comparable value is used for this purpose, i.e., 0.015. It should be pointed out that no matter what value is given for Q and H, all these parameters do not have to be changed again.

The use of a different method, DRKGS, for integrating the diffusion equation along the x direction, as compared to the eigenvalue technique utilized before, introduces one more parameter: the upper error bound, ε, as discussed by Fleischer [8]. A parametric study was performed and is shown in Figure 3.7 and Table 3.10.

Table 3.10 Computer Time Requirements for Parametric Study on ε - Elevated Point Source Model

ε	Time (sec)
$1x10^{-5}$	180
$1x10^{-6}$	190
$1x10^{-7}$	200
$1x10^{-8}$	290

The cases simulated involved meteorological parameters that exist for very unstable conditions, which will be discussed in the next section. This was done in order to have large concentration gradients and the possibility of a difficult problem to solve. The error was calculated again at the effective emission height. A two-dimensional Lagrangian

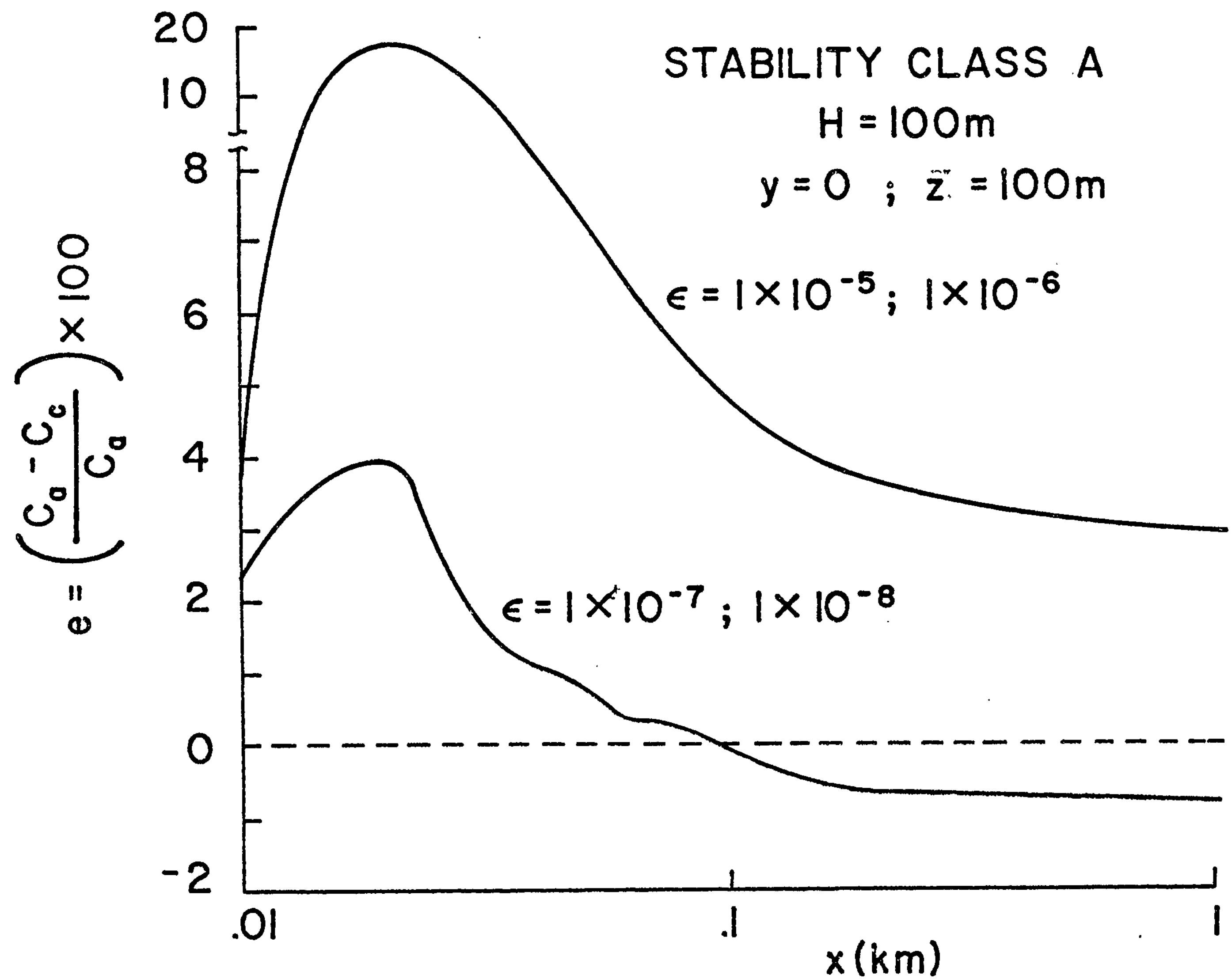

FIGURE 3.7 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT THE EFFECTIVE EMISSION HEIGHT WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY ON ϵ

interpolation, which involves the solution at all collocation points, was used. The calculated error again gives an estimate of the overall error.

An analysis of Figure 3.7 shows that the accuracy is greatly improved by modifying the upper error bound from $\varepsilon = 1\text{x}10^{-6}$ to $\varepsilon = 1\text{x}10^{-7}$, while the computer times involved are similar. The time requirements have increased very much compared to the two-dimensional cases because a system of 80 first-order ordinary differential equations is being solved for the present model.

A closer look at Figure 3.7 shows a peak in the error e at 20 m downwind from the source. For practical purposes this does not matter very much since the concentration distribution is usually desired from 50 to 100 m up downwind. Furthermore, this error is 4% which for these purposes is quite low. This peak occurs because of the large integration stepsize of 10 m at that location. A parametric study on ε with a smaller stepsize of 2.5 m was simulated next. The absolute error e was identical for all previous ε used, but not the computer time requirements which are presented in Table 3.11.

Table 3.11 Computer Time Requirements for Small Stepsize of Integration - Elevated Point Source Model

ε	Time (sec)
$1\text{x}10^{-5}$	250
$1\text{x}10^{-6}$	260
$1\text{x}10^{-7}$	270
$1\text{x}10^{-8}$	310

Since there was no dependence of ε in the error for this case, a parametric study to check r was performed again, and is shown in Figure 3.8. It can be seen that the absolute error is indeed decreased by using a smaller stepsize, and the peak is converted to a damped curve at downwind distances close to the point source. As expected and discussed before, as the ratio increased the error increased and the computer time decreased to 250 seconds ($\varepsilon = 1x10^{-7}$). The main objective of the present work is to develop a highly accurate method of solution, so the small stepsize was adopted with an upper error bound of $\varepsilon = 1x10^{-7}$.

The analysis on z_{max} discussed for the previous models still holds for the three dimensional case. It should be pointed out that an inversion layer in the lateral dimension is meaningless. Therefore, y_{max} must always be specified by the user, and if the horizontal spread of the plume has reached that value, the solution from that downwind distance until x_{max} would be erroneous. For such a case, y_{max} should be increased.

Finally, the parameters for cases with two-dimensional mean wind velocities must be specified. These cases must be treated in a different way since the concentration distribution is not symmetric to the center-line (y=0) anymore. The approach used for the vertical direction is then applied to the lateral dimension with y=0 as the analog of the effective emission height. Therefore, $N_y=N_z=10$, $\beta_y=\beta_z=.0012$, all δ are equated to .002861 and their increments to .0025.

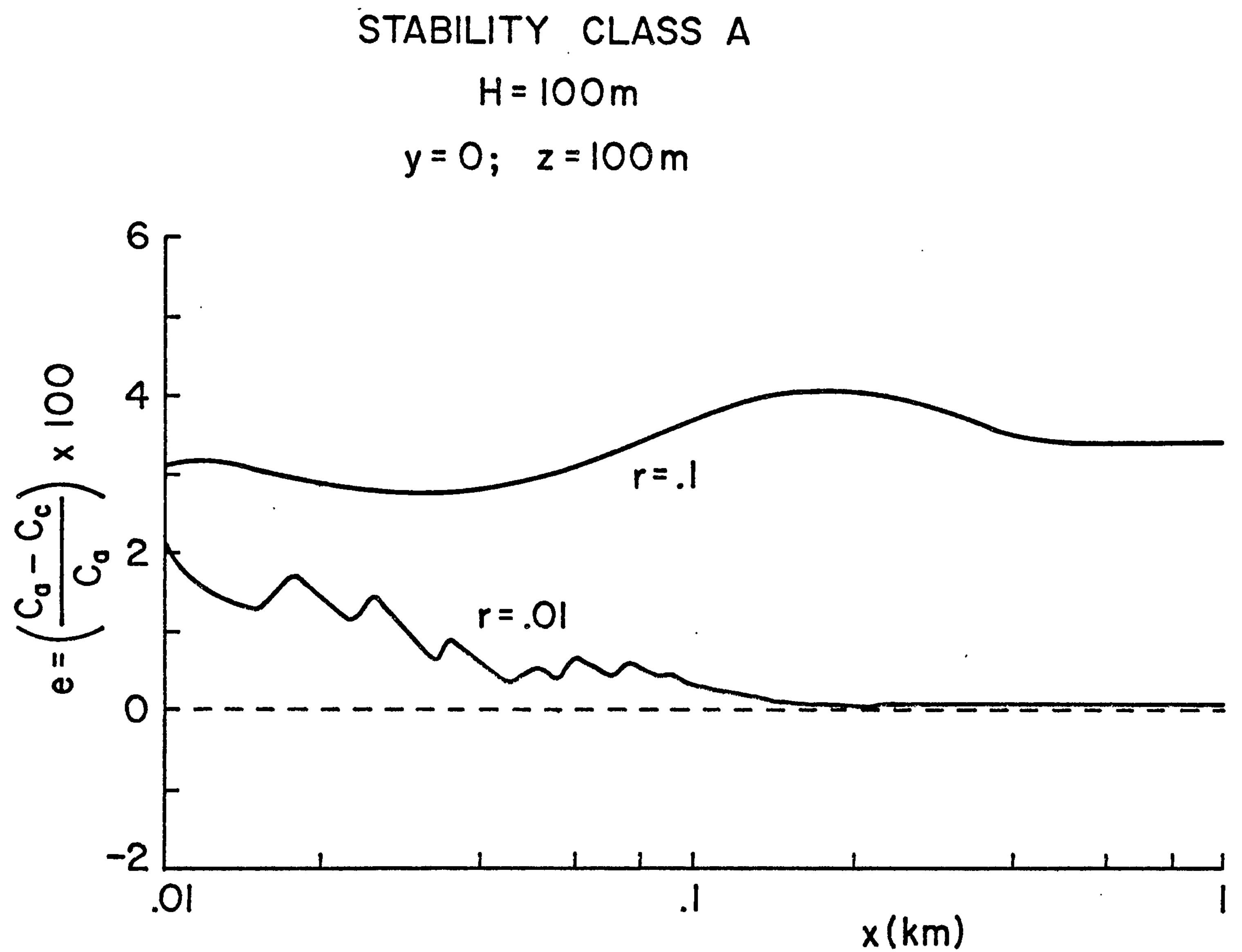

FIGURE 3.8 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT THE EFFECTIVE EMISSION HEIGHT WITH ANALYTICAL SOLUTION - PARAMETRIC STUDY OF r

Meteorological Parameters

General functional relationships and the corresponding parameters must be specified for the turbulent diffusivities and velocity profiles for completeness of the formulation of the present models. This is presented next.

Turbulent Diffusivities K_y, K_z

Any work related to air pollution modeling and dispersion processes in the atmosphere, which uses the K-theory, must include descriptions for the turbulent diffusivities in the lateral and vertical directions, K_y and K_z, respectively. Unfortunately, these descriptions vary from one work to another. Sometimes experimental data are available, but again they usually apply for the specific case in question.

Among the best of these works, Eschenroeder and Martinez [5] relate K_z to elevation and most importantly to stability classes, as defined by Pasquill and Gifford [18], a parameter that is widely used and known. The trapezoidal profile for K_z, discussed by Fleischer [8], and the values for the maximum constant vertical diffusivities from the knee height up to the inversion layer seem to describe fairly well K_z. Eschenroeder and Martinez, based on a Los Angeles tetroon data, assigned a value of 500 m^2/s for the constant horizontal diffusivity. Unfortunately, this large value, when compared to others, is not appropriate to use as a typical measure for K_y. Therefore, their description for K_z is used in the present work, but with different absolute values for K_z and K_y.

The fact that the Gaussian plume equation, which uses dispersion parameters based on experimental data, is the most widely used method to determine the concentration distribution helped to develop a method for obtaining the turbulent diffusivities. Moreover, one of the most important questions in air quality is related to the position and magnitude of the maximum ground level concentration. Therefore, the three-dimensional continuous elevated point source solution, with constant wind speed and turbulent diffusivities, was matched to the Gaussian plume equation to give the same maximum ground level concentration at the same position. The vertical diffusivity was adjusted until the position of the maximum at some downwind distance from the source was equal to the one predicted by the Gaussian plume equation. Once K_z was determined, the horizontal diffusivity was obtained when the spread of the plume was enough such that the absolute value for the maximum concentration gave the same as the Gaussian plume equation prediction. Typical values for the wind speed, depending upon stability classes, were used. Since an analytical solution for this model is available, the present method was validated by their comparison.

The resulting concentration distributions are shown in Figures 3.9 through 3.14. All cases were simulated in approximately the same computational time, i.e., 270 seconds. Excellent agreement can be observed between the concentration profiles obtained by the present technique and the analytical solution. On the other hand, except for the maximum ground level concentration, the results do not agree with the Gaussian

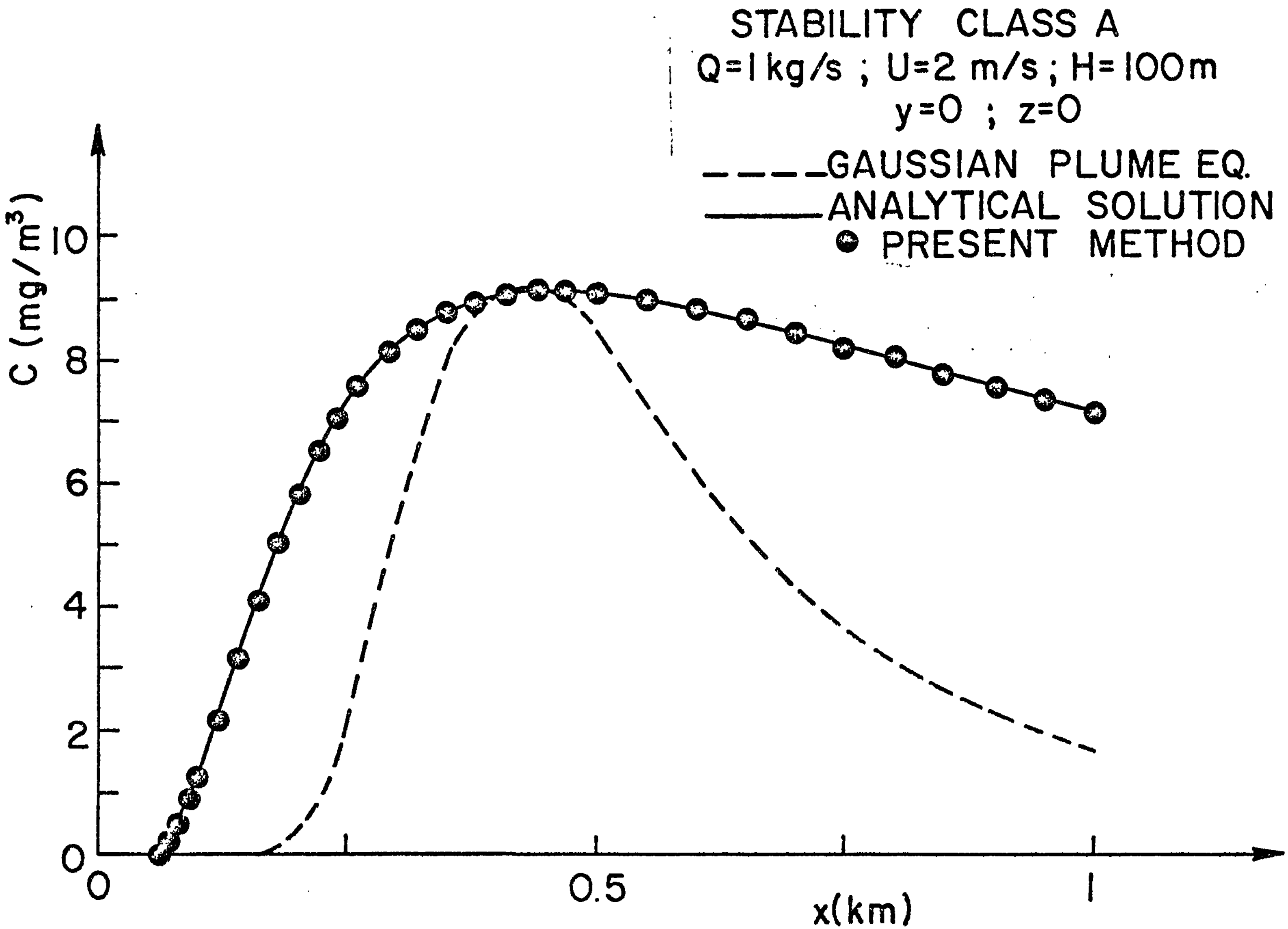

FIGURE 3.9 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS A

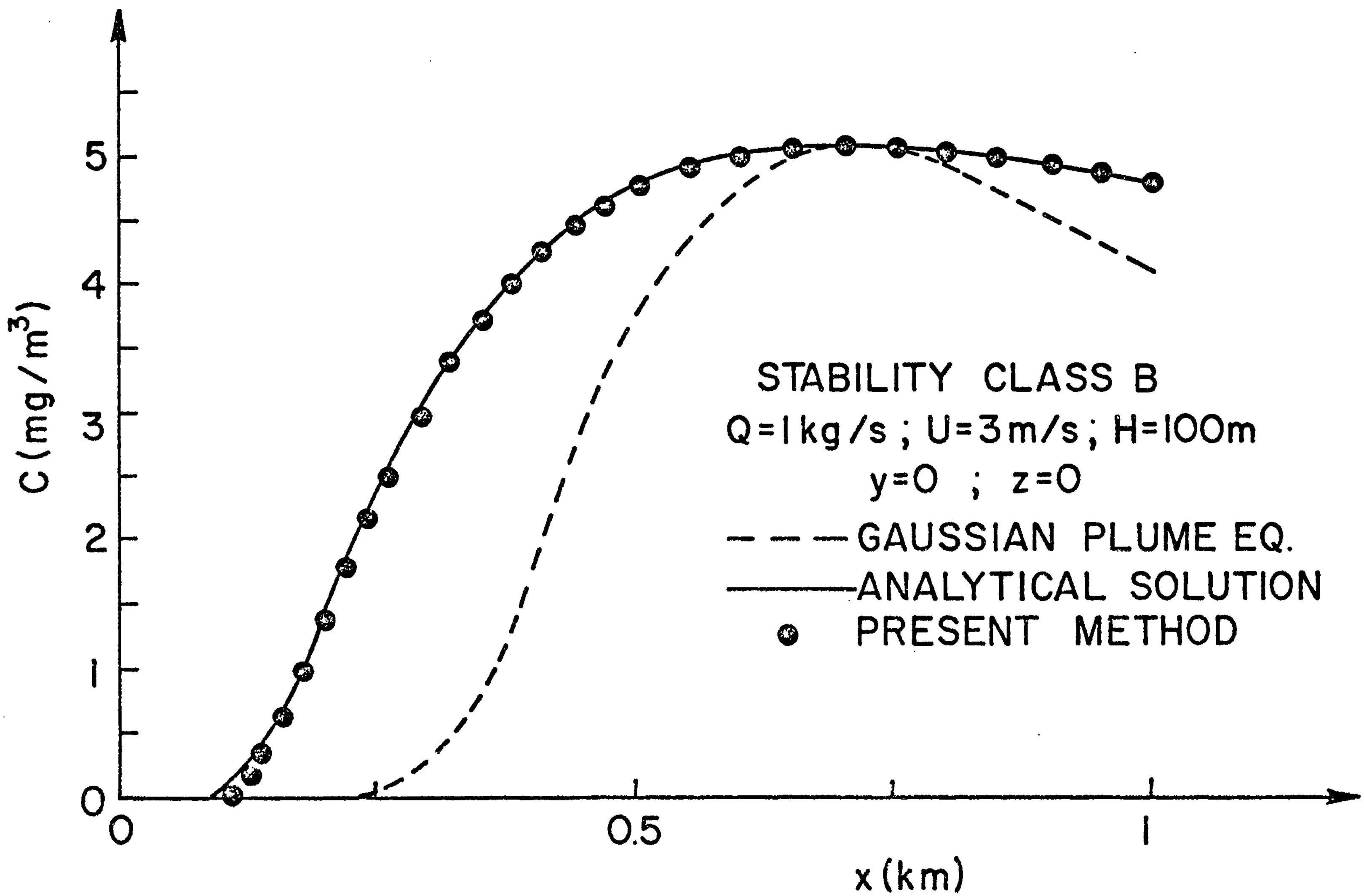

FIGURE 3.10 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS B

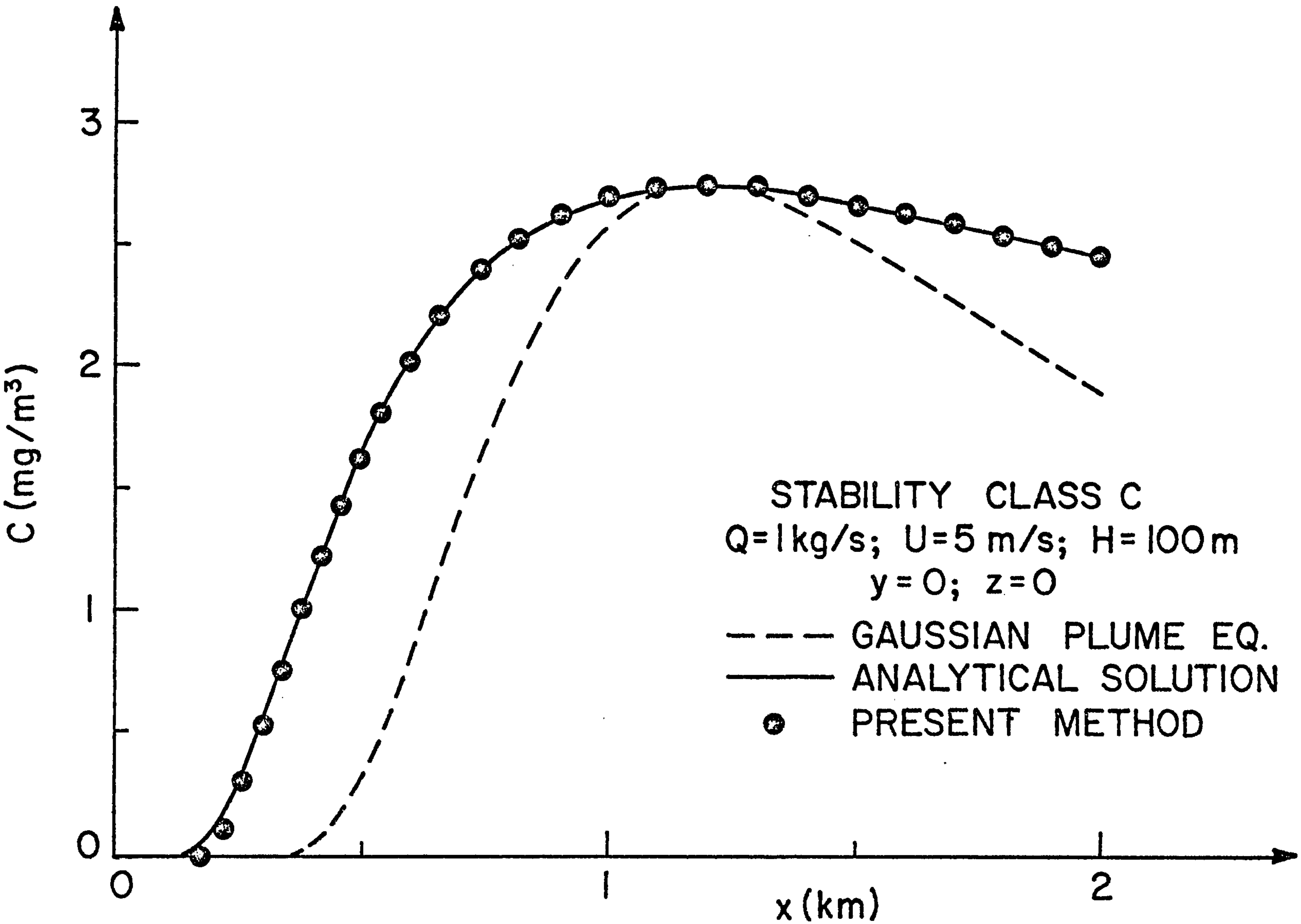

FIGURE 3.11 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS C

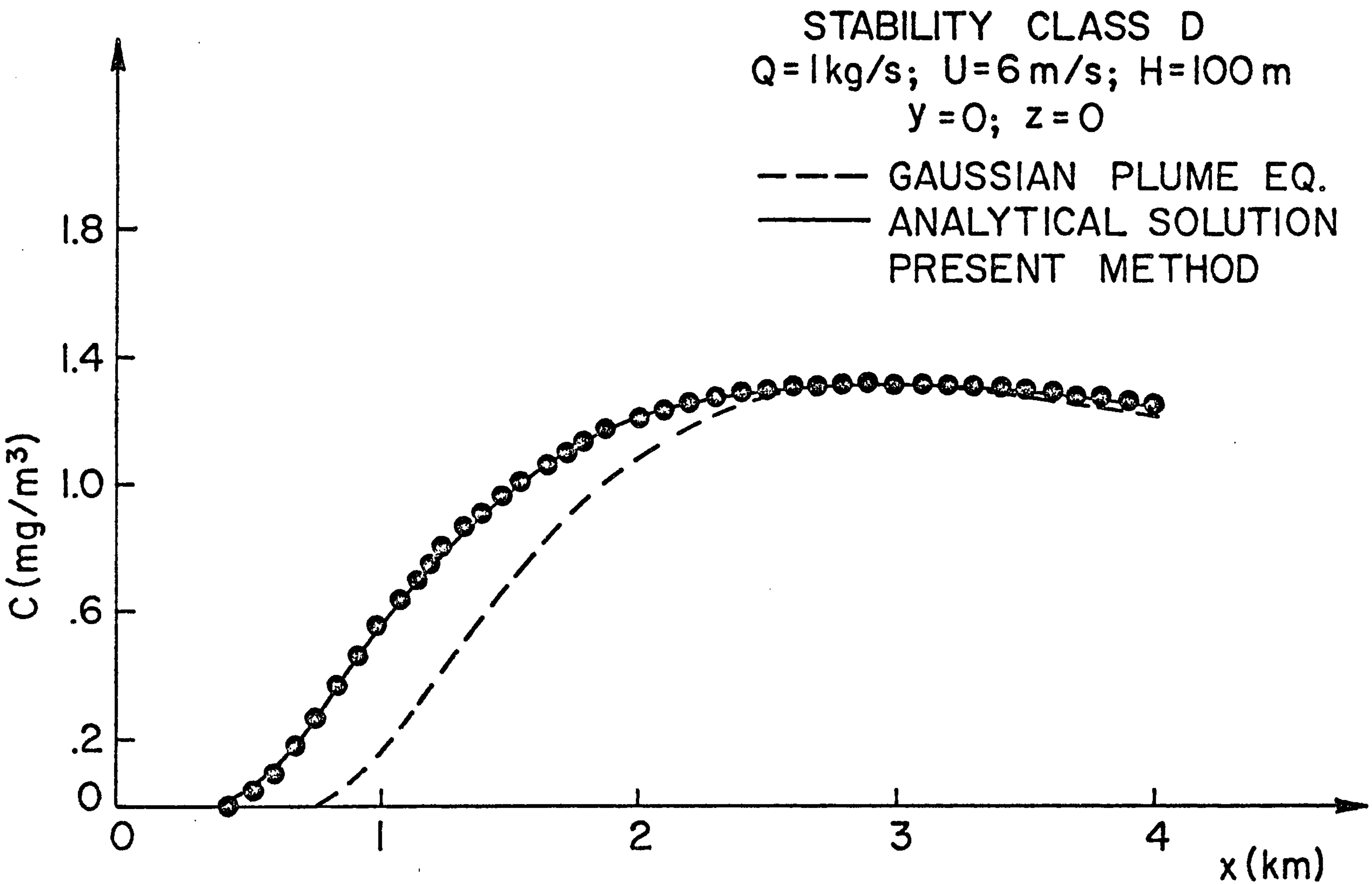

FIGURE 3.12 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS D

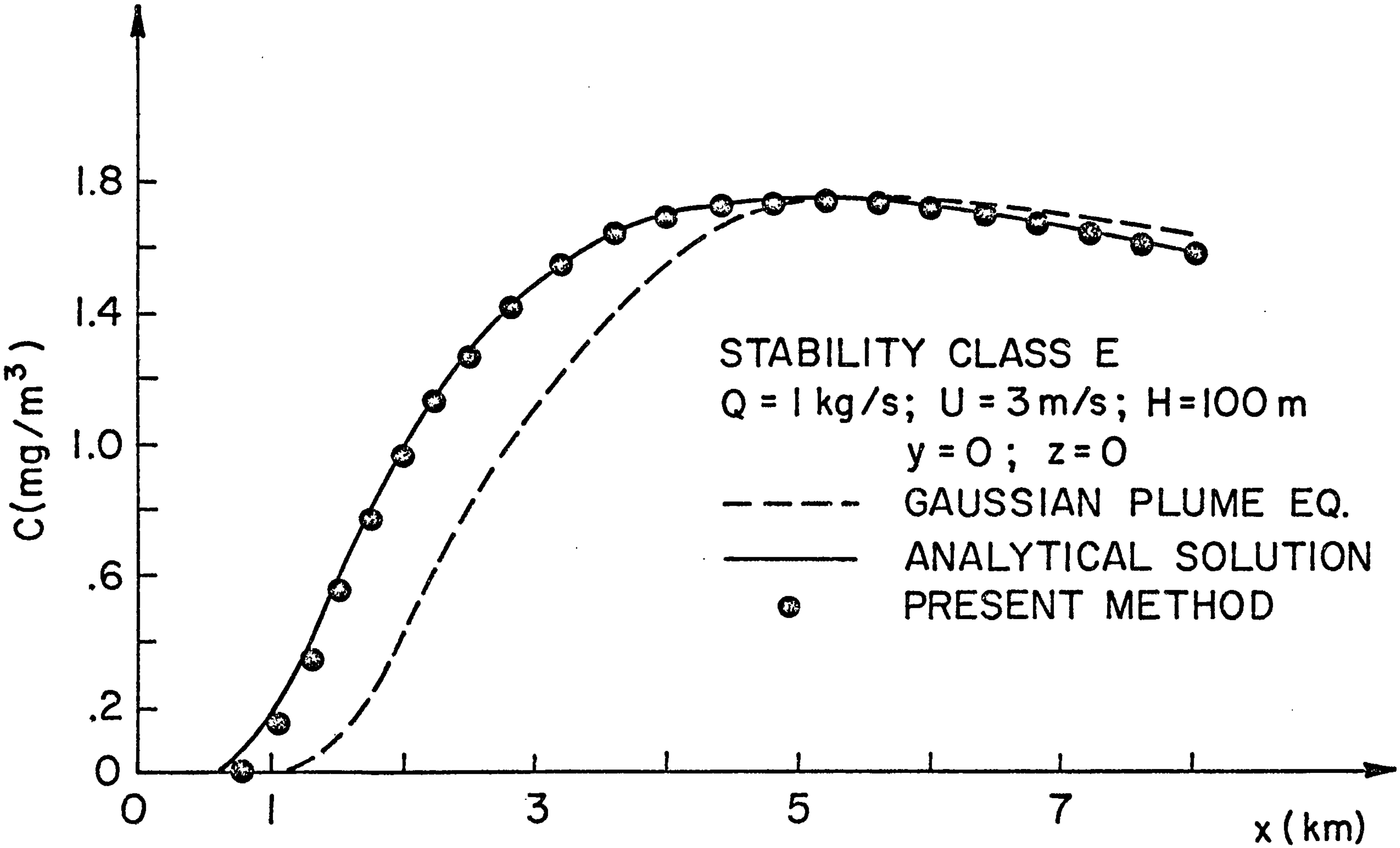

FIGURE 3.13 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS E

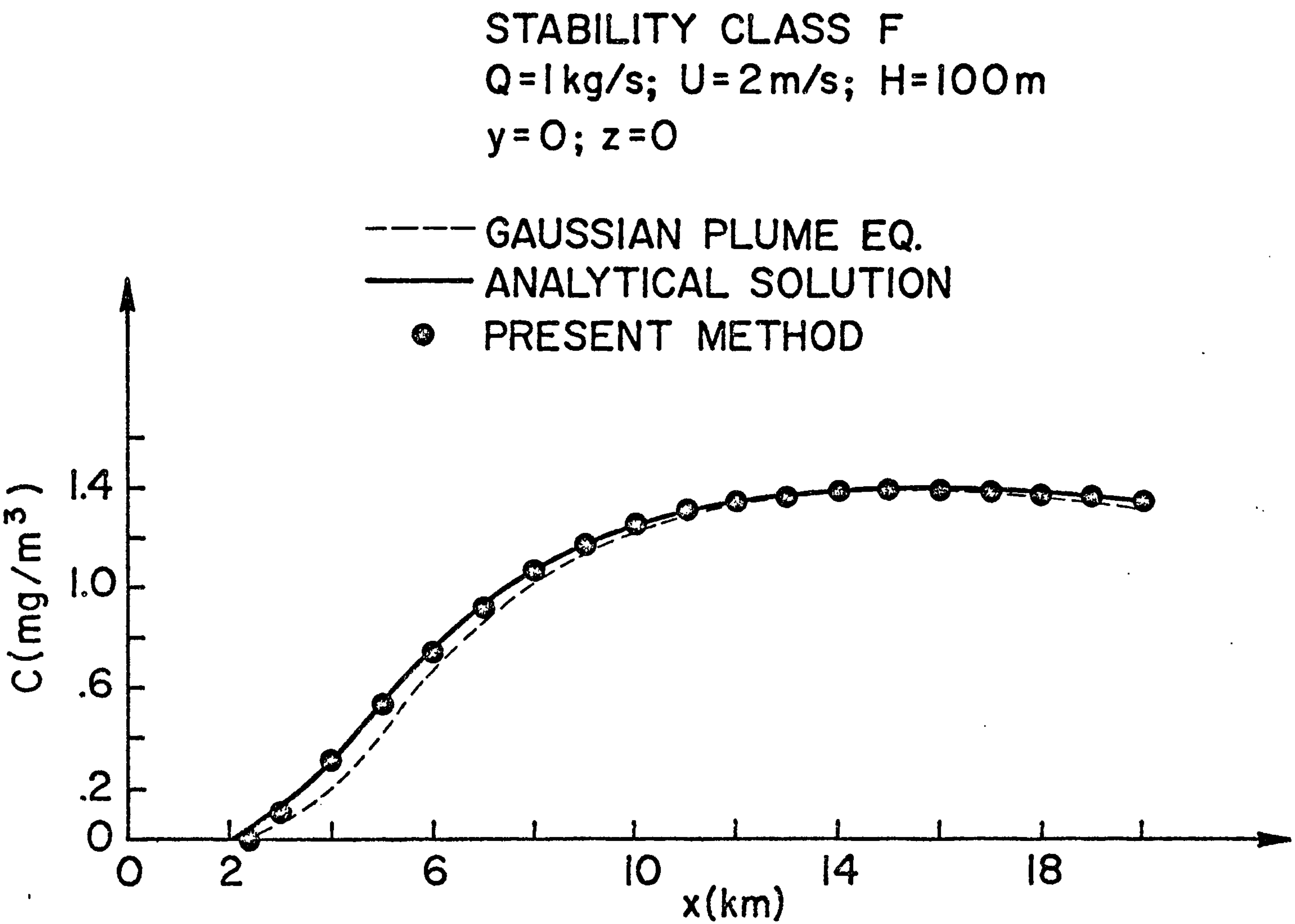

FIGURE 3.14 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS F

plume equation predictions. This is due to several reasons. The Gaussian plume equation corresponds to the solution of a simplified continuity equation assuming Gaussian distribution for the plume spread. It is a statistical method that makes use of Taylor's theorem [17] for the standard deviation, a concept which is not applied to the present technique. Furthermore the Gaussian parameters σ_y and σ_z, made functions of travelled downwind distance, were obtained and adjusted from the Project Prairie Grass field data [1,2,10] which involved a small region of interest. The pollutant was emitted at 50 cm above the ground, and most samplers were placed at 1.5 m of elevation and along semicircular arcs from 50 to 800 meters from the source. The phenomena that occur in the lower layers of the atmosphere, such as wind shear, deposition, reflection, removal, etc., and the corresponding solution should be used with caution to represent most situations. Observation of Figures 3.9 through 3.14 confirms this analysis in the sense that the more unstable the atmosphere, the larger the difference between both methods.

It should be pointed out that the present mathematical technique is valid for any type of relationship between the turbulent diffusivities and meteorological and/or spatial variables. The more complicated models are compared to the Gaussian plume equation in Chapter IV. The selection of the present procedure to determine the turbulent diffusivities was done in order to present meaningful comparisons besides lack of a reasonable algorithm. The results for the constant vertical and horizontal diffusivities obtained are presented in Table 3.12.

Table 3.12 Constant Turbulent Diffusivities and Wind Speed used in the Present Method

Stability Class	Wind Speed (m/s)	K_z (m^2/s)	K_y (m^2/s)
A	2	11	18.15
B	3	10.75	25.26
C	5	10.5	30.76
D	6	5.2	46.28
E	3	1.5	30.00
F	2	.325	22.75

Some of the results for the vertical diffusivity are in agreement with the ones presented by Eschenroeder and Martinez [5].

The values for K_y presented in Table 3.12 are then used in the present work. The ones obtained for K_z are utilized in the constant portion of the trapezoidal profile, i.e., from the knee height up to an arbitrary elevation of $(z_{max}-100)$m if $z_{max} \geq 300$m and there exists an inversion layer. If this is not the case, the constant value is used from the knee height all the way to the top. Eschenroeder and Martinez [5] use a knee height that varies from 25 to 75 meters. As suggested by Sutton [17], the surface boundary layer ends approximately at 50 meters, and therefore this is the elevation at which the knee height was put in the present work. The complete description for K_z as used in the present work, when applied as a variable with elevation, is shown in Figure 3.15.

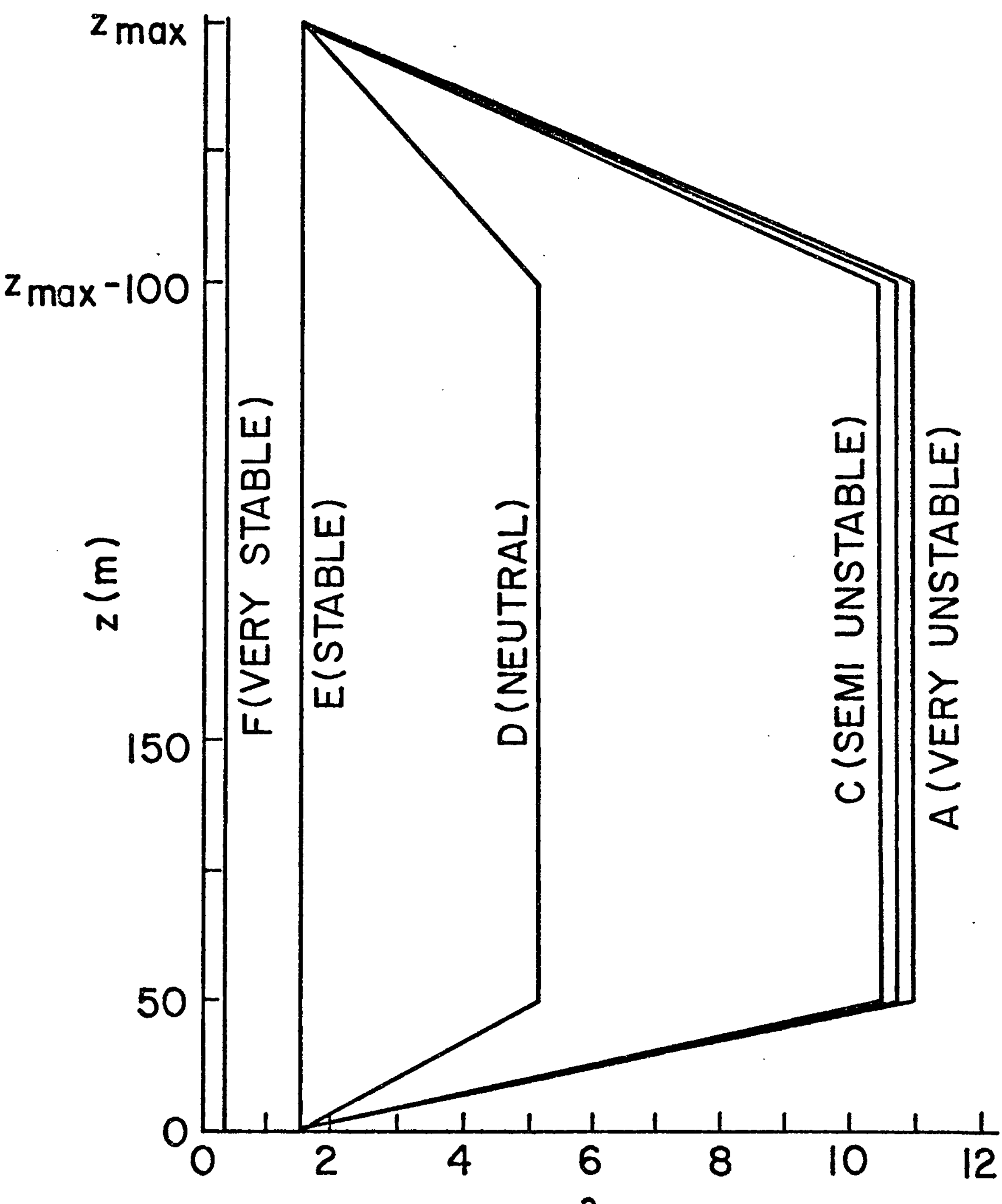

FIGURE 3.15 VERTICAL DIFFUSIVITY PROFILES IN THE PRESENT WORK

Velocity Profile

Several forms have been used to describe the one dimensional mean wind velocity [8]. They all relate u to elevation and roughness or stability classes. The power-law form is used in the present work as

$$u = u_1 \left(\frac{z}{z_1}\right)^m \tag{3.2}$$

The parameters u_1, z_1 and m should be supplied as input data by a user of the present method, although the values in Table 3.13 are given as default. Since in most cases the wind speed is known at 10 meters of elevation, z_1 is equated to this value. Furthermore, the exponent of the power-law can be related to stability classes, as presented by Seinfeld [16] and shown in Table 3.13.

Table 3.13 Estimates for the Parameters in Equation (3.2)

Stability Class	m	$u_1(z_1=10m)$ (m/s)
A	.02	2
D	.14	6
F	.83	2

At some elevation z_G called the geostrophic elevation, which is determined in the following two-dimensional wind velocity description, the mean wind velocity should become constant. Therefore, the complete specification for the one-dimensional mean wind velocity is given by

$$u = u_{10}\left(\frac{z}{10}\right)^m \qquad 0<z<z_G \tag{3.3}$$

$$u = u_{10}\left(\frac{z_G}{10}\right)^m \qquad z \geq z_G \tag{3.4}$$

The value of the velocity at the ground (z=0) is not needed in the present work since no interior collocation point will lie in a boundary, and the first and last Gaussian quadrature weights used to calculate the mass flux at any downwind position are zero.

To describe a two-dimensional wind velocity, one must analyze the phenomena that occur within the planetary boundary layer. That is, one should include the Coriolis force caused by rotation of the earth and use the basic equations of motion for two-dimensional steady mean flow, referred to axes fixed in the earth [9,13,17]:

$$f\,v - \frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{1}{\rho}\frac{\partial}{\partial z}\tau_{zx} = 0 \tag{3.5}$$

$$-f\,u - \frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{1}{\rho}\frac{\partial}{\partial z}\tau_{zy} = 0 \tag{3.6}$$

where $f = 2w \sin\phi \approx 1.458\times10^{-4} \sin\phi \ \frac{1}{\text{sec}}$ and is called the Coriolis parameter, w being the angular velocity of rotation of the earth and ϕ the geographical latitude.

By assuming that the eddy stresses are

$$\tau_{zx} = \rho K_z \frac{\partial u}{\partial z} \tag{3.7}$$

$$\tau_{zy} = \rho\ K_z \frac{\partial v}{\partial z} \tag{3.8}$$

equations (3.5) and (3.6) become

$$f\ v - \frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{\partial}{\partial z}\left(K\ \frac{\partial u}{\partial z}\right) = 0 \tag{3.9}$$

$$-f\ u - \frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{\partial}{\partial z}\left(K\ \frac{\partial v}{\partial z}\right) = 0 \tag{3.10}$$

If the x-direction is oriented parallel to the isobars, i.e. $\frac{\partial p}{\partial x} = 0$ and knowing that the free-stream velocity, called geostrophic wind u_G blows along the isobars, the velocity component perpendicular to the isobars v vanishes at the height z_G. Therefore, from equation (3.10)

$$f\ u_G = -\frac{1}{\rho}\frac{\partial p}{\partial y} \tag{3.11}$$

and equations (3.9) and (3.10) have become independent of pressure.

The Coriolis effect can usually be neglected near the surface. If this is assumed to apply from the ground up to the knee height Δ, equation (3.9) and (3.10) can be used to describe the velocity profile in the region where K_z is constant. The solution of the equations of motion is given by:

$$u = u_G(1 - e^{-az}\cos az) \tag{3.12}$$

$$v = u_G e^{-az} \sin az \tag{3.13}$$

where

$$a = \left(\frac{f}{2K_z}\right)^{\frac{1}{2}} \tag{3.14}$$

The geostrophic elevation, also used for one-dimensional velocity profiles as previously discussed, can be obtained by sutstituting v=0 into equation (3.13), i.e.,

$$z_G = \frac{\pi}{a} \tag{3.15}$$

For a Coriolis parameter of $f=10^{-4}\text{sec}^{-1}$, which corresponds to approximately a geographical latitude of 40° that occurs in the middle of the U.S., and the constant values of K_z given by Table 3.12, the resulting geostrophic elevations are presented in Table 3.14.

Table 3.14 Geostrophic Elevations used in the Present Work

Stability Class	z_G(m)
A	1475
B	1455
C	1440
D	1015
E	545
F	255

For the surface boundary layer, between the ground and the knee height Δ, the power-law form can be used for the component of the velocity in the x-direction. Since the Coriolis effect is neglected in this portion of the atmosphere, the direction of the velocity will be assumed constant and equal to the value that occurs at Δ=50m, i.e., dependent on the stability class. These values are presented in Table 3.15.

Table 3.15 Angle between Wind Velocity and Geostrophic Direction for the Surface Boundary Layer

Stability Class	α(°)
A	42
B	42
C	42
D	41
E	37
F	29

The results shown in Tables 3.14 and 3.15 are in agreement with the values suggested by Sutton [17].

The complete description for the two-dimensional wind velocity can be expressed then by the following algorithm:

$$u = u^c_{50} \left(\frac{z}{10}\right)^m \qquad \qquad (3.16)$$

$$\left.\right\} \quad \text{for } 0<z\leq\Delta$$

$$v = (\tan \alpha)u \qquad \qquad (3.17)$$

$$u = u_G(1-e^{-az} \cos az) \qquad \text{for } z>\Delta \qquad (3.18)$$

$$v = u_G e^{-az} \sin az \qquad \text{for } \Delta<z<z_G \qquad (3.19)$$

$$v = 0 \qquad \text{for } z\geq z_G \qquad (3.20)$$

where

$$u^c_{50} = u_G\left(\frac{10}{50}\right)^m (1-e^{-50a} \cos 50a) \qquad (3.21)$$

is required for a continuous velocity profile.

CHAPTER IV

PRESENTATION AND ANALYSIS OF RESULTS

The Eulerian approach was validated by Fleischer [8] through comparisons between calculated concentration distributions and the few available experimental data. The present models have been validated by comparing the calculated results with existing analytical solutions. Therefore, the main objective of the present work is to obtain concentration distributions for air pollution problems that are either difficult to simulate through conventional techniques, such as finite-differences, or which have never been solved or presented in the literature.

Two-Dimensional Models

. The first problem that was simulated includes pollutant removal from the atmosphere, represented by a simplified first order chemical reaction model, and applied to the continuous ground level line source case. The value of 1.67×10^{-3} per minute or 10% loss per hour was used as the reaction rate constant. The results, obtained in 27 seconds of CPU time, are presented in Figure 4.1. They indeed show that there is no need to include chemical reactions to a steady state model since the concentration values can be calculated by multiplying the analytical solution to the factor $\exp(-\frac{k_1 x}{u})$. This factor is the result of the chemical reaction model when solved by itself.

The other two-dimensional model simulated included an inversion layer at 250 meters for a continuous elevated line source case, with an

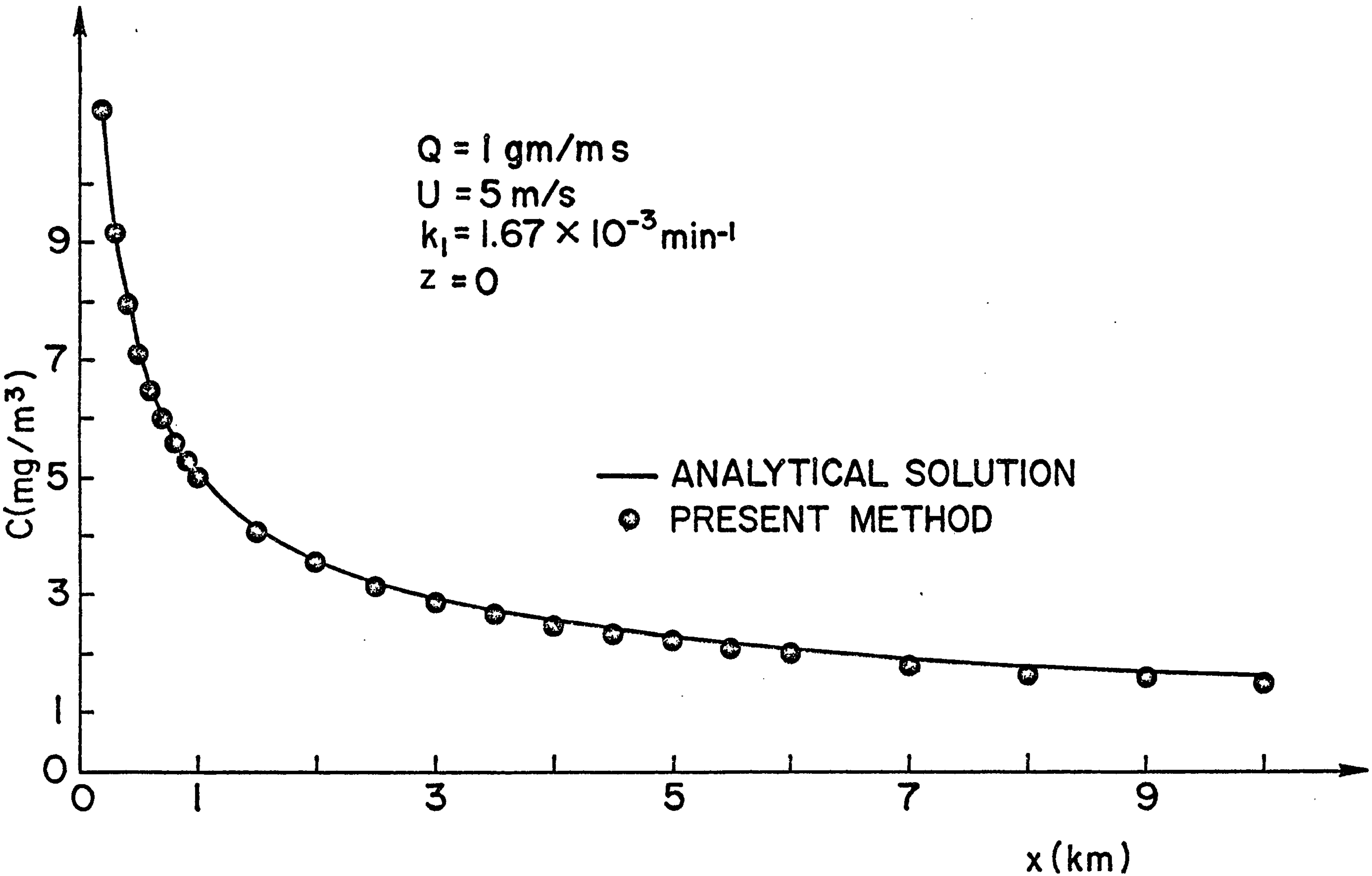

FIGURE 4.1 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - TWO DIMENSIONAL MODEL WITH CHEMICAL REACTION

effective emission height of 200 meters. The calculated and analytical concentration distributions are shown in Figure 4.2.

The results obtained from the present work in 117 seconds of CPU time predict that the plume reaches the inversion layer at a downwind distance of 300 m from the source. An inversion layer means that all the material reaching that elevation is reflected down. It can be observed that the inversion layer starts to affect the concentration at the effective emission height at about 1.5 km from the source. Since the analytical solution does not take into account the inversion layer, the calculated results are higher than the analytical solution for downwind distances over 1.5 km.

Three-Dimensional Models

There are an infinite number of situations that could be simulated by the three-dimensional models. The most representative have been selected and are presented next.

The first interesting problem is to compare the effect of having a one-dimensional wind velocity profile as a function of elevation with respect to a constant wind speed. This comparison, together with the concentration distribution obtained for the case of wind velocity and vertical turbulent diffusivity variable with elevation is shown in Figures 4.3 through 4.5. The results were obtained for the three most important stability classes, A, D, and F in approximately 260, 240, and 220 seconds of CPU time, respectively.

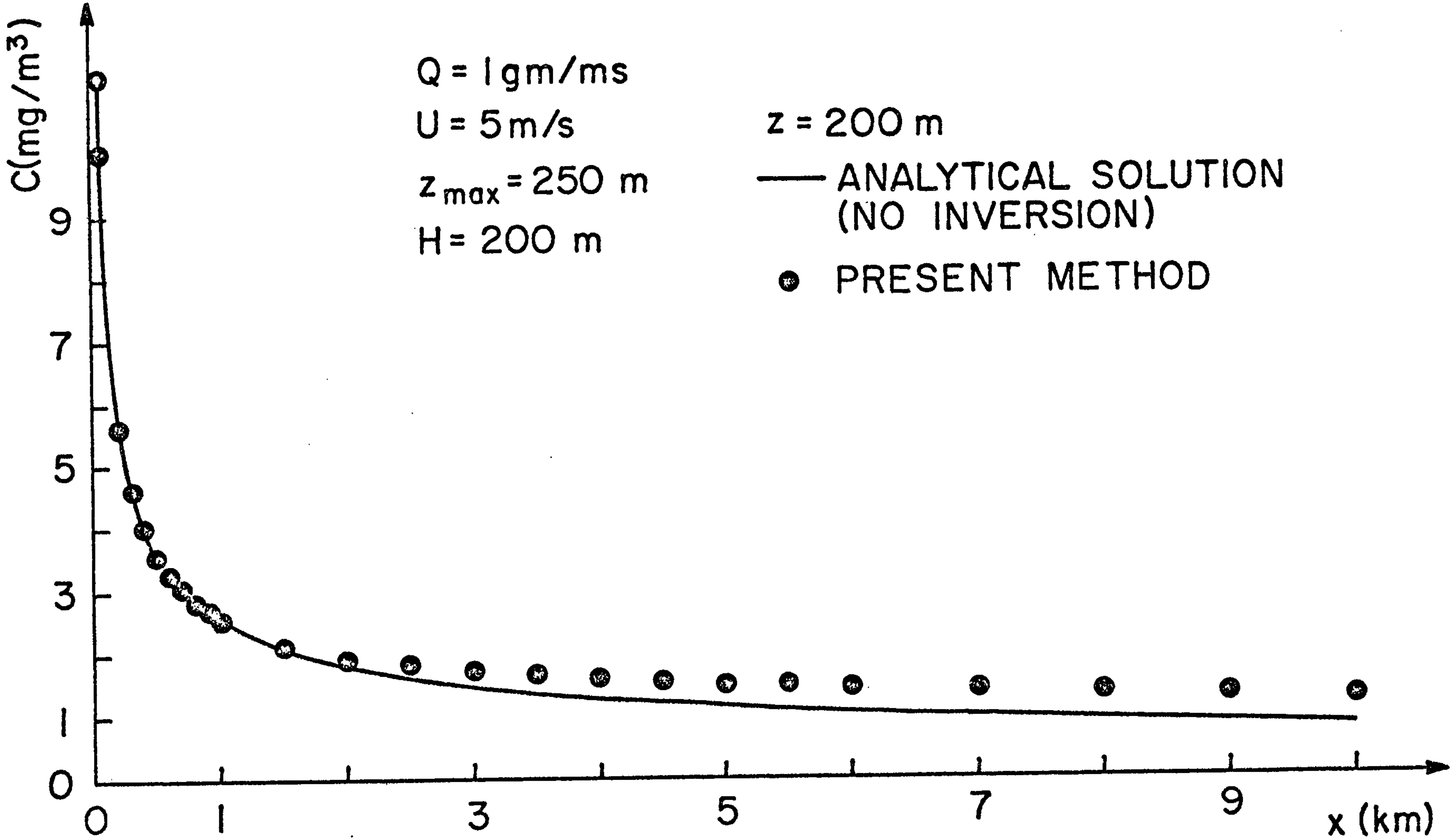

FIGURE 4.2 DOWNWIND CONCENTRATION DISTRIBUTION AT THE EFFECTIVE EMISSION HEIGHT - TWO DIMENSIONAL MODEL WITH INVERSION LAYER

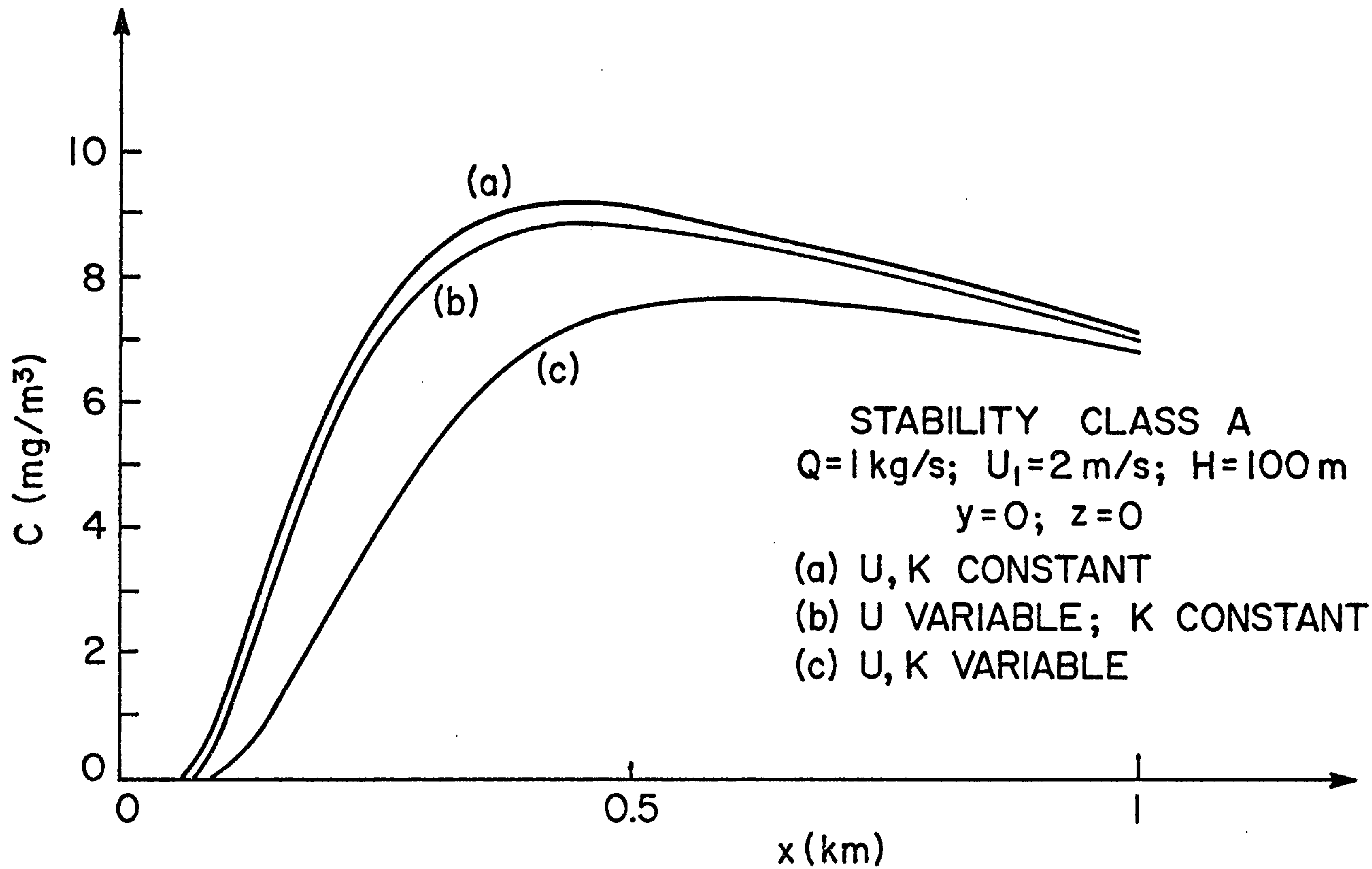

FIGURE 4.3 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - THREE DIMENSIONAL MODELS - STABILITY CLASS A

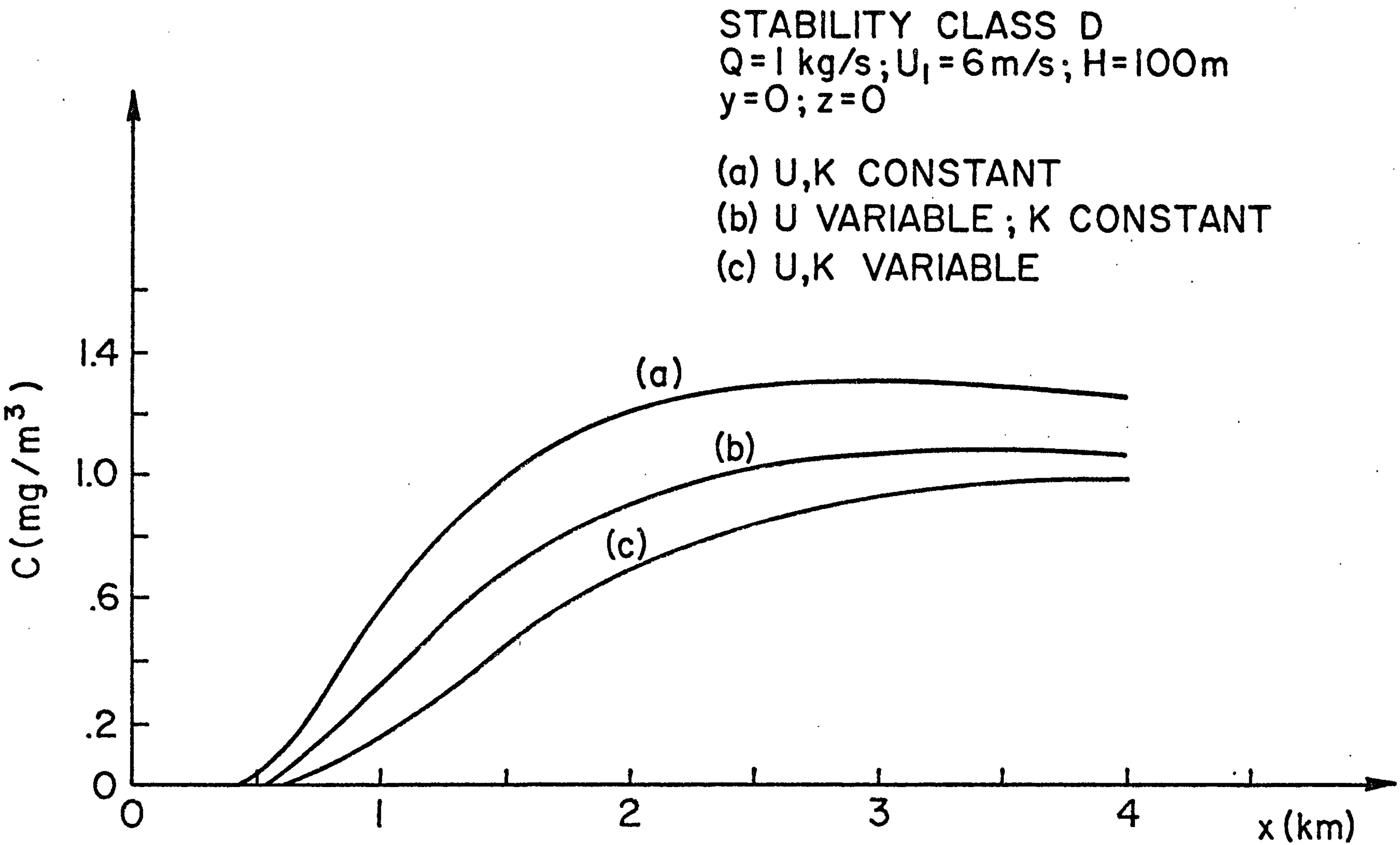

FIGURE 4.4 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - THREE DIMENSIONAL MODELS - STABILITY CLASS D

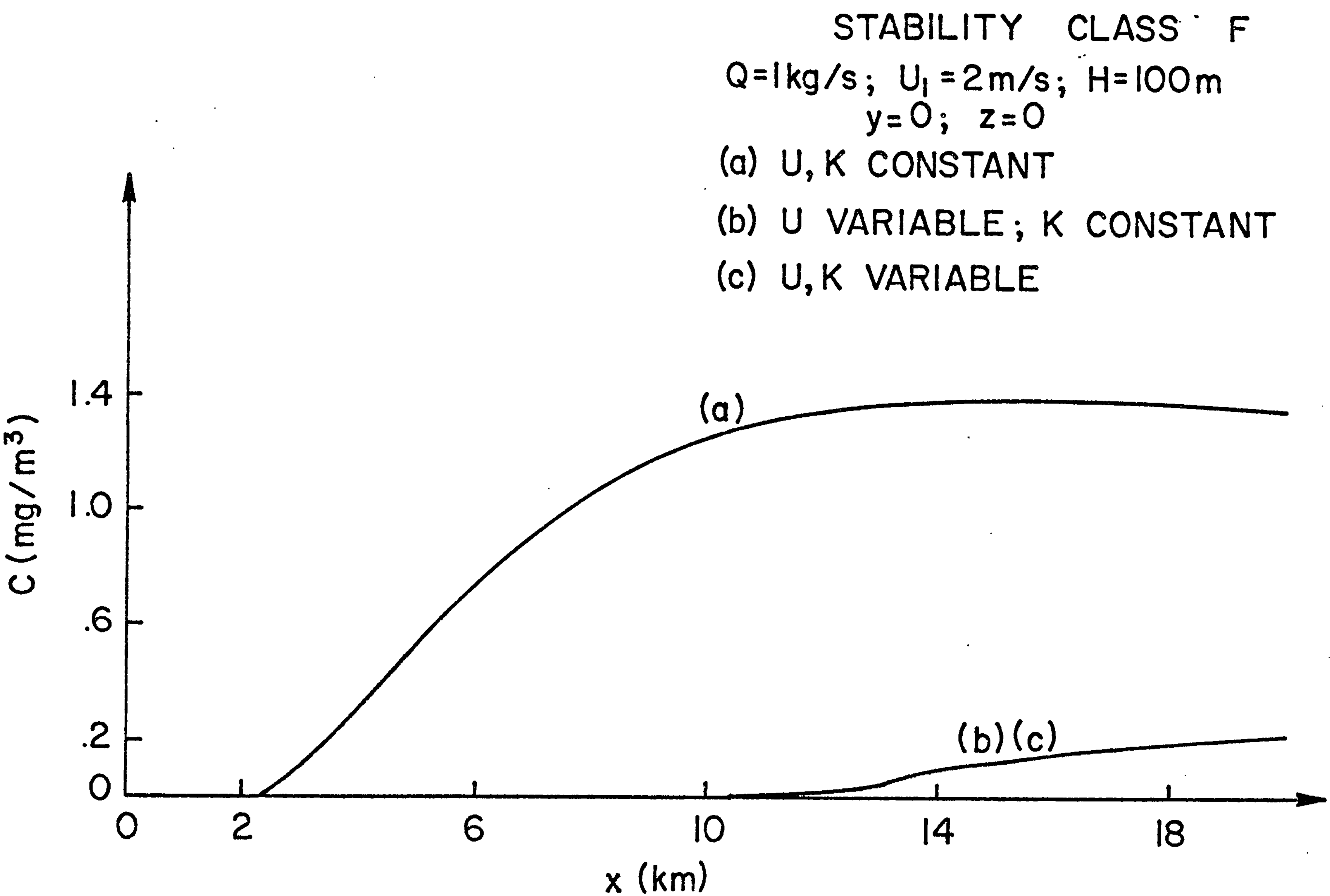

FIGURE 4.5 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - THREE DIMENSIONAL MODELS - STABILITY CLASS F

The wind speed at 10 meters, u_1 in equation (3.2), was equated to the wind speed for the constant velocity case. This means that the velocity below 10 m is lower than the constant wind speed, and that above this elevation is higher than u_1. The results, as expected, show a maximum ground level concentration lower than for the constant u and K_z model, and therefore at a larger distance downwind from the source.

The results also show the influence of the power-law exponent and the description of the variable vertical turbulent diffusivity in the ground level concentration distribution. A small value for m means that the deviation of the variable mean wind velocity with respect to the constant profile is negligible as shown by cases (a) and (b) in Figure 4.3. As m increases, the deviation from case (a) increases such that for the extreme case (very stable atmosphere, Figure 4.5) where m=.83 (Table 3.13) the concentration distribution is significantly different.

The description for the variable vertical turbulent diffusivity involves a smaller K_z, from the ground up to the knee height, when compared to the corresponding constant value. As the instability of the atmosphere increases, this constant K_z increases and the difference between cases (b) and (c) in Figures 4.3 and 4.4 is magnified. An extreme case is again a stability class F (Figure 4.5), where no difference exists between variable and constant turbulent diffusivity, and therefore cases (b) and (c) lie in the same curve.

The Gaussian plume equation is the most widely used model in air pollution since the concentration can be obtained in a very simple way. Figure 4.6, extracted from Turner [18], shows the ease with which the ground

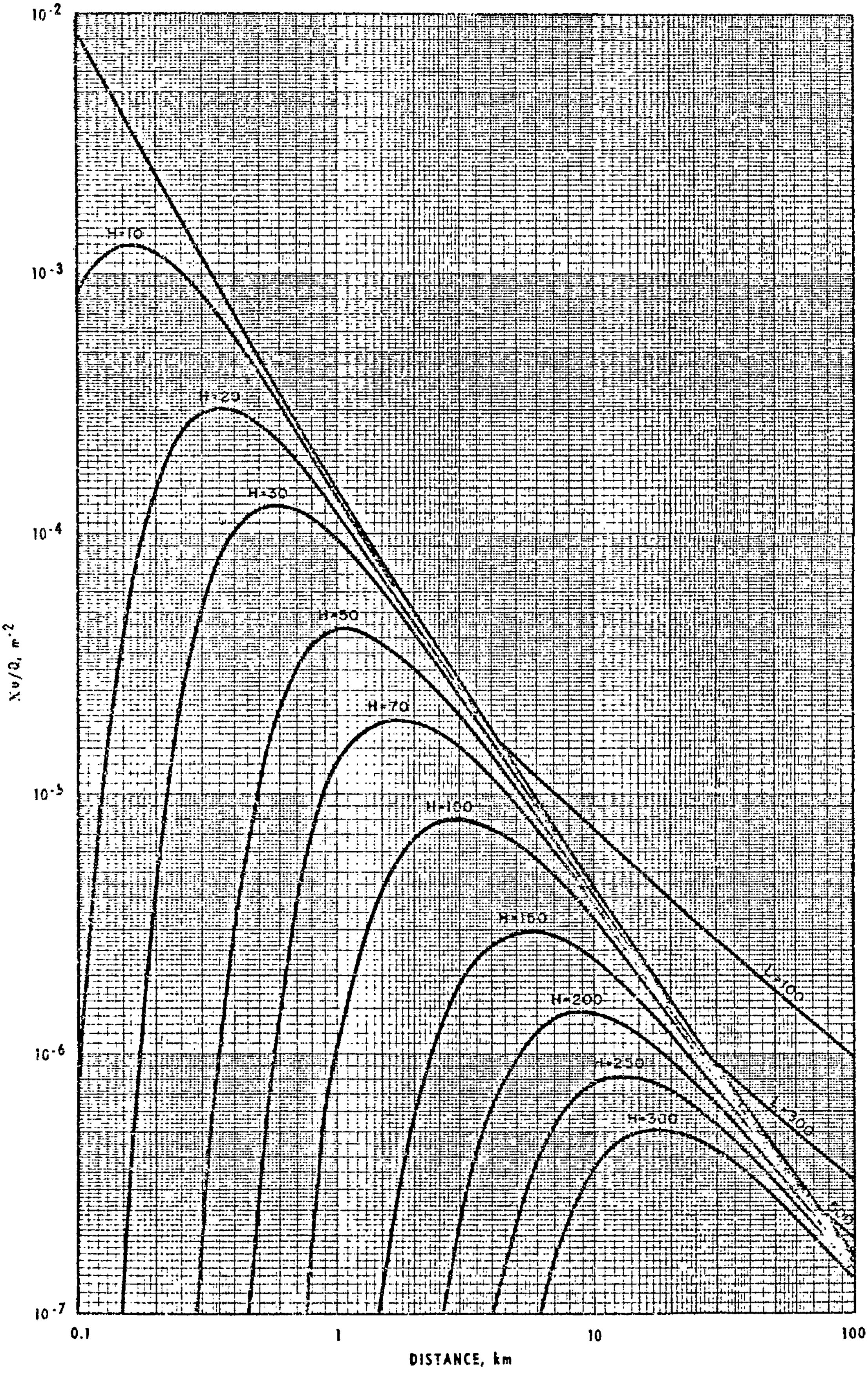

FIGURE 4.6 $\frac{\chi U}{Q}$ WITH DOWNWIND DISTANCE FOR VARIOUS HEIGHTS OF EMISSION - GAUSSIAN PLUME EQUATION

level concentration can be obtained for any emission rate Q, wind speed U, effective emission height H, and stability class. Unfortunately, this model should be used only for homogeneous and stationary conditions, with all the restrictions discussed in Chapter III.

A graphical method, similar to the one discussed above, is developed in the present work for estimation of ground level concentration for the several Pasquill-Gifford stability classes. The present computed results were obtained for a wind velocity profile which obeys equations (3.3) and (3.4), a vertical turbulent diffusivity represented by Figure 3.15, and K_y given by Table 3.12.

The main difference of the present model and the Gaussian plume equation is that the position of the maximum ground level concentration depends on the wind speed, as it should. Therefore, the variable plotted in the abscissa is the time of flight $\frac{x}{u_1}$ and not x.

The results, for stability class D, are shown in Figure 4.7.

The next more complex three-dimensional model which is solved in the present work incorporates a two-dimensional wind velocity profile. In order to validate the present results, a constant wind direction case was solved first, such that an analytical solution could be available.

A continuous point source emitting 1 kg/s of material at an effective emission height of 100 m into a neutral atmosphere (constant diffusivities) with a constant axial velocity of 6 m/s and a lateral wind speed of 3 m/s in the negative y-direction was simulated using the present technique. The results are compared to the analytical solution with a constant wind speed of the resultant velocity, i.e., 6.71 m/s. The concentration

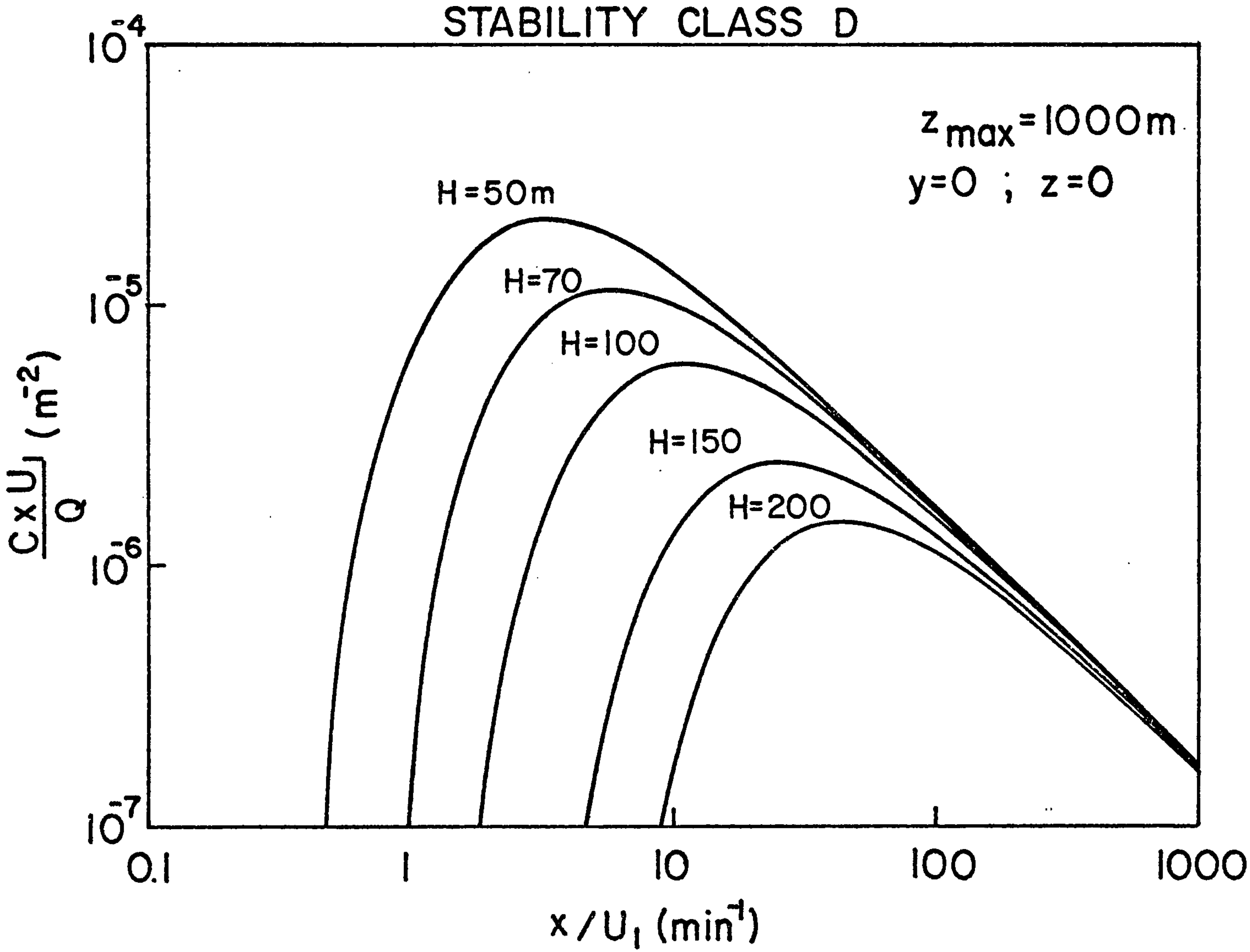

FIGURE 4.7 $\frac{Cu_1}{Q}$ WITH TRAVEL TIME FOR VARIOUS HEIGHTS OF EMISSION - PRESENT WORK

distribution at ground level and at the effective emission height are presented in Figure 4.8. The agreement is excellent. It should be pointed out that again the concentration at z=100 m is obtained through two-dimensional Lagrangian interpolation, and therefore shows the overall error involved in the computed results. The computer time was 800 seconds.

With the present work validated for the case of a two-dimensional wind velocity profile, the next step was to solve the problem with the Coriolis effect. The wind velocity was represented by equations (3.16) through (3.21) and the vertical diffusivity profile by Figure 3.15. The constant horizontal diffusivity was given by Table 3.12. The geostrophic velocity was taken to be the same as u_G given by the power-law equation, with u_1 for a stability class D assumed to be equal to 6 m/s. A value of u_G = 11.45 m/s was calculated for these conditions.

Isopleths of 3 mg/m^3 for the present model and the constant wind speed and turbulent diffusivity are shown in Figure 4.9. Both cases are quite different, as expected. The centerline for case (a) occurs at y=0 while for case (b) is skewed to the left. Furthermore, the areas are different but the mass flux is the same, i.e., 1 kg/s. The reason being that in general, the concentrations for the constant case are higher than for the Coriolis model, e.g., the maximum concentrations found were 5.36 mg/m^3 and 5.00 mg/m^3, respectively. The peculiar form of the curve at the left, i.e., more voluminous is due to the effect that the isopleth has reached the ground and the material is being reflected upwards.

Figure 4.10 shows the comparison of the Coriolis model to the Gaussian plume equation for the ground level concentration at both

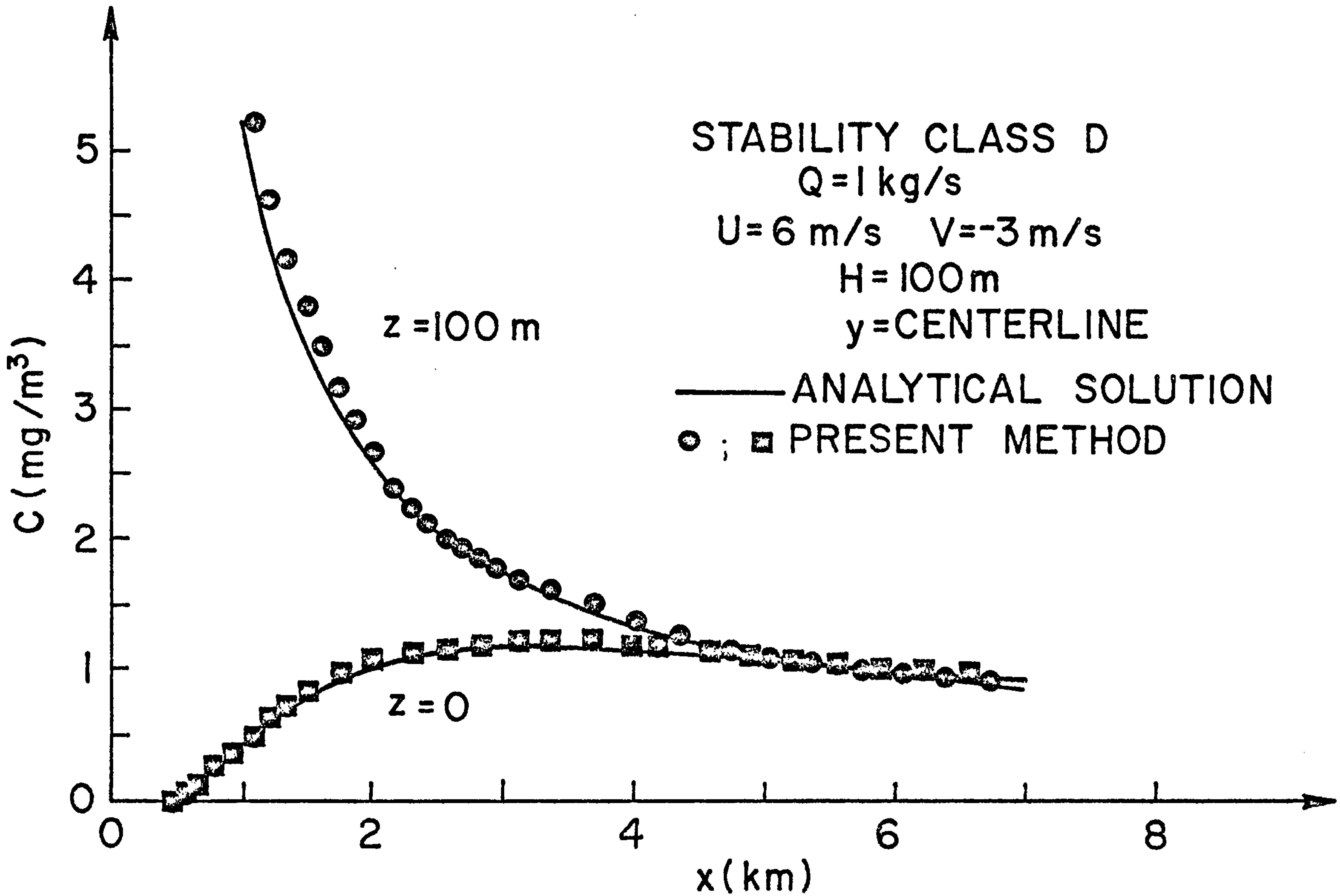

FIGURE 4.8 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION WITH ANALYTICAL SOLUTION - TWO DIMENSIONAL WIND VELOCITY

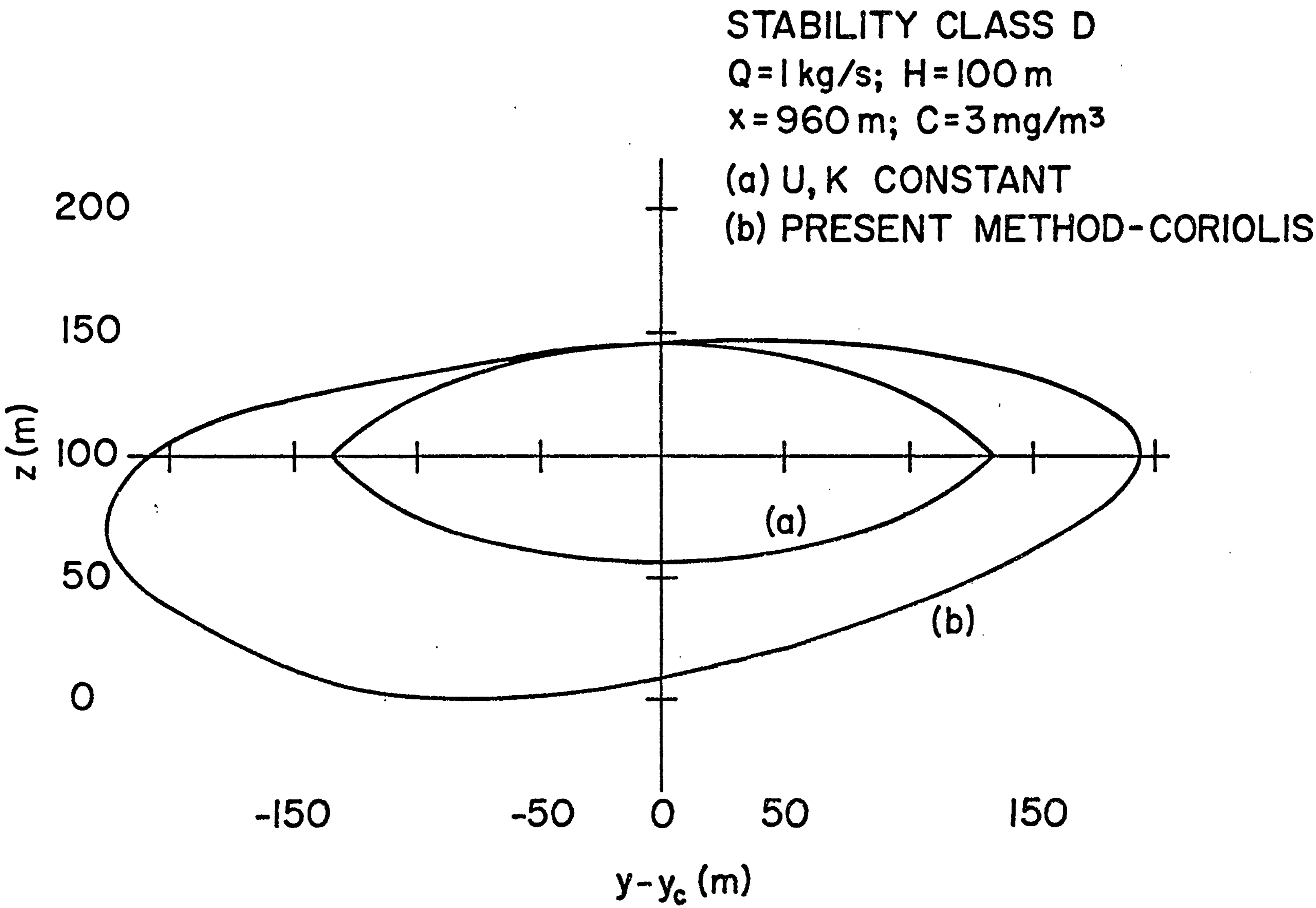

FIGURE 4.9 ISOPLETHS AT A CONSTANT x - THREE DIMENSIONAL MODELS

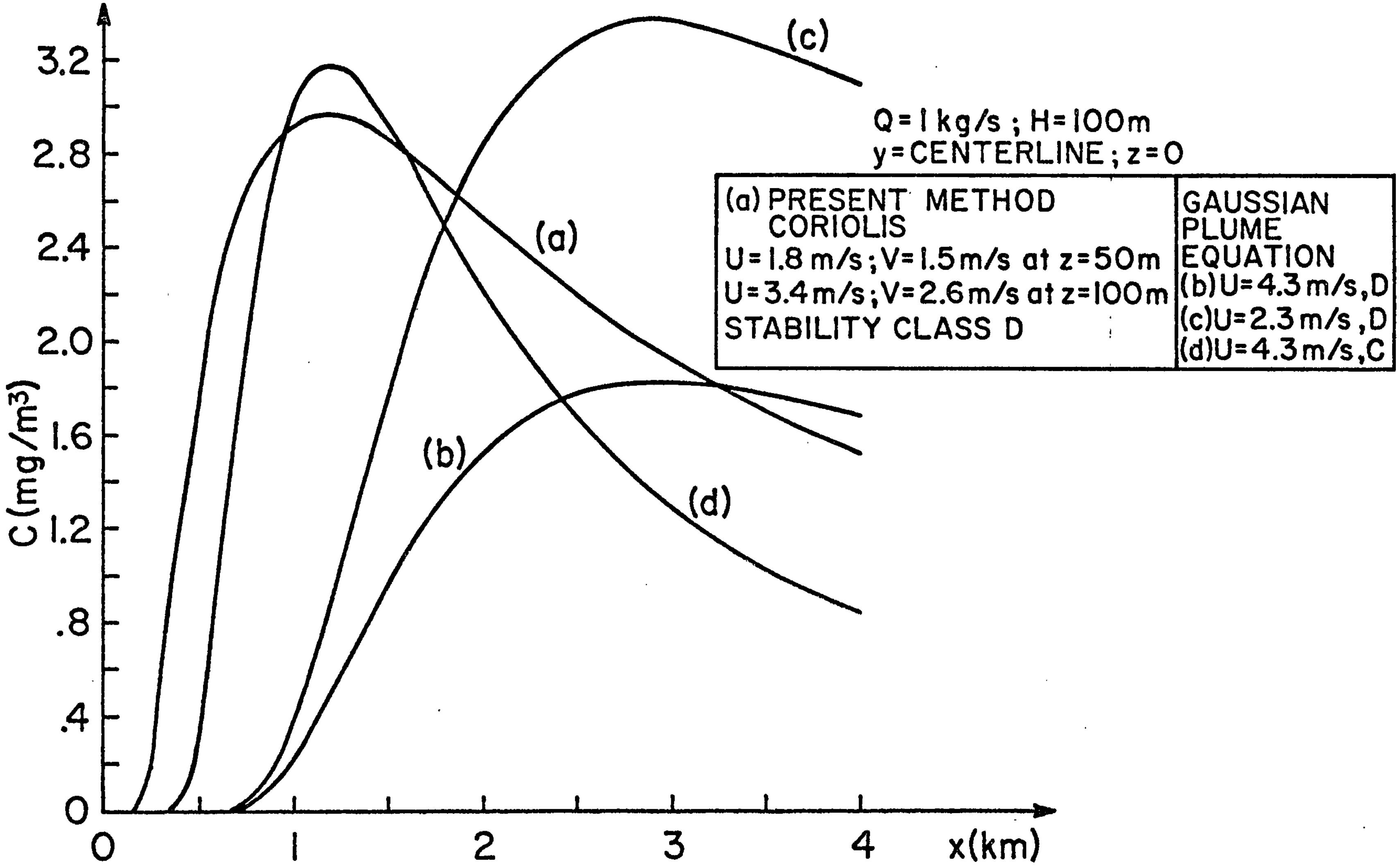

FIGURE 4.10 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - CORIOLIS EFFECT VS GAUSSIAN PLUME EQUATION

centerlines. Cases (b) and (c) were obtained for a wind speed equal to the resultant of the velocity for the present model at the effective emission height, 100 m, and at an elevation of 50 meters, respectively. The three cases were obtained for neutral stability, and the results are quite different.

Since the wind speed used for case (b) is 4.3 m/s, it would be more appropriate to obtain the solution using the Gaussian plume equation for a stability class C. This concentration distribution is also shown in Figure 4.10 as case (d), and the comparison to the present model is closer, at least in the downwind position and the value of the maximum ground level concentration. For the wind speed of 2.3 m/s no stability class was found that would give a Gaussian plume equation solution closer to the present model.

It should be noted, as has extensively been done before, that less rigorous mathematical parameters can provide a decrease in the computational time. The Coriolis model case (a) was obtained in 880 seconds of CPU time. A similar problem was simulated next, but the mathematical parameter r was changed to 0.1. A comparison of the mass fluxes at several downwind positions is shown in Table 4.1.

Table 4.1 Mass Rates at Several Downwind Positions - Coriolis Effect

x(m)	Q_x(kg/s)	
	r = .01	r = .1
10	1.0026	1.0031
20	1.0011	1.0108
50	1.0003	.9990
100	1.0067	.9759
200	1.0054	.9881
500	.9976	.9902
960	.9992	1.0348
2000	.9874	.9973
4000	.9846	.9768

It can be observed that the results for the case with r = 0.1(Q=1 kg/s) are still adequate as compared to the simulation using r = 0.01, but the main difference lies in the computer time involved of 580 seconds.

CHAPTER V

SUMMARY OF RESULTS, CONCLUSIONS AND RECOMMENDATIONS

Turbulent diffusion from single ground level or elevated line or point sources in the atmosphere was successfully simulated using the K-theory and solved by spline orthogonal collocation. Improved mathematical techniques were used to describe the plume, which is generated at the source, by means of moving boundary conditions. This implies that the edges of the plume are known at any downwind distance from the source, and the concentration distribution is obtained only within the region of interest, i.e., in the plume. Although the solution was calculated at the orthogonal collocation points, accurate two-dimensional Lagrangian interpolation was used to obtain the concentration at other desired positions such as the effective emission height.

Several techniques for solving the resulting system of first-order ordinary differential equations with respect to the along wind direction were tested in the present work. An eigenvalue method was selected for the two-dimensional models, and the three-dimensional models were solved by a fourth-order Runge-Kutta method.

The present work was used to simulate steady state air pollution models. Mathematical parameters, inherent of the techniques developed, were determined through parametric studies. The values assigned for these mathematical parameters should remain unchanged if the present work is used for other problem specifications.

Empirical equations were used to describe the mean wind velocity and the turbulent diffusivities. Several meteorological parameters were included in these equations so that many atmospheric conditions can be simulated by the present technique. A two-dimensional wind velocity profile, including the Coriolis effect, obtained by solving the equations of motion analytically, was incorporated in the three-dimensional air pollution model.

Excellent agreement was observed between the calculated concentration distribution and the analytical solution for cases where the latter exists. The present model had also an excellent response to variations in atmospheric conditions. This was obtained by simulating hypothetical cases. In addition to the concentration distribution, the flux across any plane normal to the along wind direction was calculated. Its comparison to the constant emission rate (steady-state models, no removal processes) was excellent. All the results were obtained with a very reasonable amount of computer time. This computational time could have been decreased by changing some mathematical parameters, but it was decided not to do so in order to obtain very accurate results. A graphical method for presenting computed results was developed to permit estimation of ground level concentration for any source emission rate, wind velocity and effective emission height for neutral stability.

Several extensions to the present technique should be investigated and are recommended next. They cover a wide spectrum of air pollution problems and do not involve significant changes to the present method.

1) Solution of pollutant dispersion from multiple sources in the atmosphere can be obtained by superposition of the effects of the individual plumes [4]. This involves only bookkeeping of the solutions in the computer. The present method required approximately 20 and 30K of storage for the two and three-dimensional models, respectively, leaving enough room for solving this type of problem. It should be pointed out that the CPU time would be the one used in the present work multiplied by the number of sources involved. If the number of sources is very large it might be more convenient, timewise, to treat them as area sources and use finite-difference as the numerical technique.

2) There is sometimes a need for solving air pollution models involving complex terrain such as buildings, hills, etc. The idea of a vertical moving boundary, similar to the one used in the present work, but fixed to the description of the terrain could be used to solve this type of problem.

3) Finally, unsteady-state models are of some interest in air pollution modeling. Sources with emission rates as functions of time, problems involving complex removal processes and/or meteorological parameters variable with respect to time are typical examples of situations that are represented by unsteady-state models.

An unsteady-state model was tried using the present technique. It required the solution of 800 first-order ordinary differential equations at each time-step of integration. The method was abandoned because it involved an excessive amount of CPU time.

Experimental data for time-changing emissions and also meteorological conditions are usually given in time intervals of one hour or higher. This suggests then to utilize a "quasi-steady-state" assumption. A solution using the present model could be obtained and applied to some interval of time, comparable to x_{max}/u. Each interval could be assumed sufficiently long to permit full development of the concentration distribution at all locations. This could be a poor approximation at low wind speeds. The extreme case studied in the present work, the very stable atmosphere, involved a time interval of approximately 2 hours for the maximum downwind distance considered significant. The general unsteady-state situation could then be obtained through a sequence of steady-state intervals. In general, both the pollutant emission and the meteorological conditions could then be varied between the consecutive time periods.

Finally, air pollution models involving complex removal processes could be treated in a similar way. The chemical kinetic terms generally require smaller time steps for stability when compared to advection time steps. This suggests then to separate the solution of the removal processes from the diffusion equation for any advection time step. The present method could be used to obtain the concentration distribution for a time step equivalent to $\Delta x/u$, Δx being the integration step in the downwind direction. The chemistry would then be calculated until the chemical time equals the advection time. The process of first calculating advection and then incorporating the chemistry solution could be repeated as long as desired. This splitting technique has been used by Eskridge and Demerjian [6,7] and by Rizzi and Bailey [15].

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A P P E N D I C E S

APPENDIX A

COMPUTER PROGRAM LISTING

Part of the computer program used for the three-dimensional - Coriolis effect model is shown next. The main programs for the other models and the subroutines common to all of them can be obtained from the Chemical Engineering Department at the University of Houston. All statements are written in Fortran IV. These programs have been executed in IBM 360/44 and UNIVAC 1108 digital computers.

```
C     ************************************************************************
C
C     THREE DIMENSIONAL MODEL WITH CORIOLIS EFFECT
C
C     DEVELOPED BY MIGUEL T. FLEISCHER
C
C     ************************************************************************
C
C
C     NOMENCLATURE
C
C        AKYB,AKZB     - TURBULENT DIFFUSIVITIES
C        ALPHA         - CONSTANT TO DETERMINE THE HORIZONTAL DIFFUSIVITY
C        AM,AMM        - CONSTANTS USED IN THE VELOCITY PROFILES
C        BETAY,BETAZ   - MATHEMATICAL PARAMETERS IN MODEL
C        CBX           - EQUIVALENT SOURCE CONCENTRATION
C        C(Y,Z)        - MEAN CONCENTRATION AT Y AND Z
C        DKN(ISTB)     - KNEE HEIGHT FOR AKZB
C        DUN(ISTB)     - REFERENCE HEIGHT FOR POWER-LAW VELOCITY PROFILE
C        D1Y,....,D2Z  - MATHEMATICAL PARAMETERS IN MODEL
C        DD1Y,..,DD2Z  - INCREMENTS OF THE PREVIOUS PARAMETERS
C        HGEO(ISTB)    - GEOSTROPHIC ELEVATION
C        HSKN          - IF GT H, NO SECOND KNEE HEIGHT FOR AKZB
C        ISTB          - STABILITY CLASS (1 VERY UNSTABLE, 6 VERY STABLE)
C        NY,NZ         - NUMBER OF COLLOCATION POINTS IN Y,Z DIRECTIONS
C        QS            - SOURCE STRENGTH
C        RATIO         - RATIO OF BOUNDARY TO CENTERLINE CONCENTRATION
C        SEL           - EFFECTIVE EMISSION HEIGHT (LIMITS 0 TO 1)
C        U,V           - WIND VELOCITY IN X,Y DIRECTIONS
C        UGR           - VELOCITY AT GROUND LEVEL
C        US            - VELOCITY AT THE EFFECTIVE EMISSION HEIGHT
C        UST           - GEOSTROPHIC VELOCITY
C        WY,WZ         - QUADRATURE WEIGHTS
C        X,X0,DX       - DOWNWIND DIRECTION, INITIAL VALUE, INCREMENT
C        XMAX,YMAX,H   - MAXIMUM DISTANCES IN X,Y,Z DIRECTIONS
```

```
C     Y,Z            - LATERAL AND VERTICAL DIRECTIONS
C
      IMPLICIT REAL*8(A-H,O-Z)
      EXTERNAL FCT
      DIMENSION FAY(12),FAZ(12),FB(12),FC(12),RTY(12),RTZ(12),
     1AY(12,12),BY(12,12),AZ(12,12),BZ(12,12),WY(12),WZ(12),
     2VEC(12),A1Y(12),A2Y(12),A1Z(12),A2Z(12),AVY(12,12),
     3Y(12),Z(12),AKY(12,12),AKZ(12,12),DAKZ(12,12),ACTY(12),ACTZ(12),
     4YINTP(12),ZINTP(12),P(100),CECO(12),EHCO(12),CECCY(12),
     5C(12,12),CC(12,12),PW(100,100),
     6PRMT(5),DY(100),AUX(8,100),DKN(6),DUN(6),HGEO(6),
     7R1(12),R2(12),R3(12),R5(12),R6(12),AKYB(12),AKZB(12),DAKZB(12),
     8U(12),V(12)
C
C     READ AND WRITE INPUT DATA
C
      READ(5,100) NY,NZ,ISTR
  100 FORMAT(3I5)
      READ(5,101) XMAX,H,YMAX,ALPHA,AK
  101 FORMAT(5D15.4)
      READ(5,106) UST,AM,UGR,QS,SEL
  106 FORMAT(5D15.4)
      READ(5,98) (DKN(I), I=1,6)
   98 FORMAT(6D10.1)
      READ(5,99) (DUN(I), I=1,6)
      READ(5,99) (HGEO(I), I=1,6)
   99 FORMAT(6D10.1)
      READ(5,104) (PRMT(I), I=1,4)
  104 FORMAT(4D15.4)
      READ(5,102) D1Y,D2Y,RATIO,BETAY
      READ(5,1020) D1Z,D2Z,BETAZ
  102 FORMAT(4D15.4)
 1020 FORMAT(3D15.4)
      READ(5,103) XC,DX,DD1Y,DD2Y
      READ(5,102) DD1Z,DD2Z,HSKN,AMM
  103 FORMAT(4D15.4)
```

```
      WRITE(6,105) (PRMT(I), I=1,4)                                     MAIN 720
  105 FORMAT(10(/),20X,'PRMTS =',4(E15.4,10X))                          MAIN 730
      WRITE(6,400) XMAX,YMAX,H,SEL,UST,UGR,AM,AMM,QS,ALPHA,AK,XO,DX,    MAIN 740
     1RATIO,BETAY,BETAZ,D1Y,D2Y,D1Z,D2Z,DD1Y,DD2Y,DD1Z,DD2Z,NY,NZ,ISTB, MAIN 750
     2DKN(ISTB),DUN(ISTB),HSKN,HGEO(ISTB)                               MAIN 760
  400 FORMAT(2(/),20X,'XMAX =',F15.4,10X,'YMAX =',F15.4,10X,            MAIN 770
     1'H =',F15.4,10X,'SEL =',F15.4,2(/),20X,'UST =',F15.4,10X,         MAIN 780
     2'UGR =',F15.4,10X,'AM =',F15.4,2(/),20X,'AMM =',F15.4,10X,        MAIN 790
     3'QS =',F15.4,10X,'ALPHA =',F15.4,10X,'AK =',E15.4,2(/),           MAIN 800
     420X,'XO =',E15.4,10X,'DX =',E15.4,10X,'RATIO =',E15.4,10X,        MAIN 810
     52(/),20X,'BETAY =',E15.4,10X,'BETAZ =',E15.4,                     MAIN 820
     62(/),20X,'D1Y =',E15.4,                                           MAIN 830
     710X,'D2Y =',E15.4,10X,'D1Z =',E15.4,10X,'D2Z =',E15.4,2(/),       MAIN 840
     820X,'DD1Y =',E15.4,5X,'DD2Y =',E15.4,10X,'DD1Z =',E15.4,5X,       MAIN 850
     9'DD2Z =',E15.4,2(/),20X,'NY =',I3,9X,'NZ =',I3,9X,'ISTB =',I3,2(/)MAIN 860
     *,20X,'DKN =',F15.4,10X,'DUN =',F15.4,10X,'HSKN =',F15.4,10X,      MAIN 870
     *'HGEO =',F15.4,/)                                                 MAIN 880
C                                                                       MAIN 890
C     INITIALIZATION                                                    MAIN 900
C                                                                       MAIN 910
      IOKYP=0                                                           MAIN 920
      IOKYM=0                                                           MAIN 930
      IIOKY=0                                                           MAIN 940
      IST=0                                                             MAIN 950
      HSEL=SEL*H                                                        MAIN 960
      DMULY=1.D0                                                        MAIN 970
      DMULZ=1.D0                                                        MAIN 980
      D10Y=D1Y                                                          MAIN 990
      D10Z=D1Z                                                          MAIN1000
      D20Y=D2Y                                                          MAIN1010
      D20Z=D2Z                                                          MAIN1020
      NTY=NY+2                                                          MAIN1030
      N1Y=NY+1                                                          MAIN1040
      NTYH=NTY/2                                                        MAIN1050
      NTYH1=NTYH+1                                                      MAIN1060
      NTZ=NZ+2                                                          MAIN1070
```

```
      N1Z=NZ+1                                                          MAIN1080
      NDIM=NY*NZ                                                        MAIN1090
C                                                                       MAIN1100
C     CALCULATION OF ORTHOGONAL POINTS, QUADRATURE WEIGHTS,             MAIN1110
C     AND MATRICES A AND B                                              MAIN1120
C                                                                       MAIN1130
      CALL JCOBI(12,NY,1,1,0.0D0,0.0D0,FAY,FB,FC,RTY)                   MAIN1140
      CALL DFOPR(12,NY,1,1,I,3,FAY,FB,FC,RTY,WY)                        MAIN1150
      DO 457 I=1,NTY                                                    MAIN1160
      CALL DFOPR(12,NY,1,1,I,1,FAY,FB,FC,RTY,VEC)                       MAIN1170
      DO 2 K=1,NTY                                                      MAIN1180
    2 AY(I,K)=VEC(K)                                                    MAIN1190
      CALL DFOPR(12,NY,1,1,I,2,FAY,FB,FC,RTY,VEC)                       MAIN1200
      DO 3 K=1,NTY                                                      MAIN1210
    3 BY(I,K)=VEC(K)                                                    MAIN1220
  457 CONTINUE                                                          MAIN1230
      CALL JCOBI(12,NZ,1,1,0.0D0,0.0D0,FAZ,FB,FC,RTZ)                   MAIN1240
      CALL DFOPR(12,NZ,1,1,I,3,FAZ,FB,FC,RTZ,WZ)                        MAIN1250
      DO 458 I=1,NTZ                                                    MAIN1260
      CALL DFOPR(12,NZ,1,1,I,1,FAZ,FB,FC,RTZ,VEC)                       MAIN1270
      DO 222 K=1,NTZ                                                    MAIN1280
  222 AZ(I,K)=VEC(K)                                                    MAIN1290
      CALL DFOPR(12,NZ,1,1,I,2,FAZ,FB,FC,RTZ,VEC)                       MAIN1300
      DO 333 K=1,NTZ                                                    MAIN1310
  333 BZ(I,K)=VEC(K)                                                    MAIN1320
  458 CONTINUE                                                          MAIN1330
      NS=NY*NZ                                                          MAIN1340
      X=X0                                                              MAIN1350
C                                                                       MAIN1360
C     INITIAL CONDITION DETERMINATION                                   MAIN1370
C                                                                       MAIN1380
      CALL VELDIF(Z,H,UGR,UST,AM,U,V,ISTB,ALPHA,NTZ,AKYB,AKZB,DAKZB,    MAIN1390
     1SEL,C,US,DKN,DLN,HSKN,HGEO,AMM)                                   MAIN1400
     PV=-UST*DEXP(-SEL*H/AM)*DSIN(SEL*H/AM)/US                          MAIN1410
     CDX=QS/8.D0/US/YMAX/H/BETAY/BETAZ                                  MAIN1420
     DO 26 J=1,NZ                                                       MAIN1430
```

```
      DO 26 I=1,NY
      JJ=I+(J-1)*NY
      PP=1.0D0
      IF((D1Y+D2Y+2.D0*BETAY)*RTY(I+1)-D1Y) 29,28,27
   29 P(JJ)=0.0D0
      GO TO 26
   28 PP=0.5D0
      GO TO 299
   27 IF((D1Y+D2Y+2.D0*BETAY)*RTY(I+1)-D1Y-2.D0*BETAY) 299,298,297
  297 P(JJ)=0.0D0
      GO TO 26
  298 PP=0.5D0
      GO TO 299
  299 IF((D1Z+D2Z+2.D0*BETAZ)*RTZ(J+1)-D1Z) 39,38,37
   39 P(JJ)=0.0D0
      GO TO 26
   38 P(JJ)=0.5D0*CBX
      GO TO 26
   37 IF((D1Z+D2Z+2.D0*BETAZ)*RTZ(J+1)-D1Z-2.D0*BETAZ) 36,35,34
   34 P(JJ)=0.0D0
      GO TO 26
   35 P(JJ)=0.5D0*CBX
      GO TO 26
   36 P(JJ)=CBX*PP
   26 CONTINUE
C
C     CALCULATION OF EXPRESSIONS USED IN MODEL (DEPENDENT
C     OF THE NUMBER OF COLLOCATION POINTS ONLY)
C
      DENY=AY(NTY,1)*AY(1,NTY)-AY(1,1)*AY(NTY,NTY)
      DO 41 I=2,N1Y
      A2Y(I)=AY(1,1)*AY(NTY,I)-AY(NTY,1)*AY(1,I)
      A1Y(I)=AY(1,I)+AY(1,NTY)*A2Y(I)/DENY
   41 CONTINUE
      DENZ=AZ(NTZ,1)*AZ(1,NTZ)-AZ(1,1)*AZ(NTZ,NTZ)
      DO 441 I=2,N1Z
```

```
      A2Z(I)=AZ(1,1)*AZ(NTZ,I)-AZ(NTZ,1)*AZ(1,I)
      A1Z(I)=AZ(1,I)+AZ(1,NTZ)*A2Z(I)/DENZ
  441 CONTINUE
C
C     LOOP FOR CHANGING THE BOUNDARY POSITIONS
C
   20 CONTINUE
      VAR1Y=DABS(D1Y+BETAY-.5DC)
      VAR2Y=DABS(D2Y-1.D0+.5D0+BETAY)
      VAR1Z=DABS(D1Z+BETAZ-SEL)
      VAR2Z=DABS(D2Z-1.DC+SEL+BETAZ)
      WRITE(6,506) D1Y,D2Y,D1Z,D2Z
  506 FORMAT(5(/),10X,'D1Y =',F10.7,5X,'D2Y =',F10.7,10X,
     1'D1Z =',F10.7,5X,'D2Z =',F10.7,1(/))
      DO 8 I=1,NTY
      Y(I)=(D1Y+D2Y+2.D0*BETAY)*RTY(I)+.5D0-BETAY-D1Y
    8 ACTY(I)=(2.D0*Y(I)-1.DC)*YMAX
      DO 888 I=1,NTZ
      Z(I)=(D1Z+D2Z+2.D0*BETAZ)*RTZ(I)+SEL-BETAZ-D1Z
  888 ACTZ(I)=Z(I)*H
      RSEL=(BETAZ+D1Z)/(D1Z+D2Z+2.DC*BETAZ)
      RYC=(BETAY+D1Y)/(D1Y+D2Y+2.D0*BETAY)
      ARYC=(2.DC*0.5D0-1.D0)*YMAX
C
C     CALCULATION OF THE DIFFERENTIAL EQUATIONS COEFFICIENTS
C
      CALL VELDIF(Z,H,UGR,UST,AM,U,V,ISTB,ALPHA,NTZ,AKYB,AKZB,DAKZB,
     1SEL,1,US,DKN,DUN,HSKN,HGEC,AMM)
      DO 2500 L=2,N1Z
      R1(L)=U(L)/XMAX
      R2(L)=V(L)/2.DC/YMAX/(D1Y+D2Y+2.DC*BETAY)
      R3(L)=DAKZB(L)/H/(D1Z+D2Z+2.D0*BETAZ)
      R5(L)=AKYB(L)/4.D0/YMAX/YMAX/(D1Y+D2Y+2.DC*BETAY)**2
      R6(L)=AKZB(L)/H/H/(D1Z+D2Z+2.D0*BETAZ)/(D1Z+D2Z+2.DC*BETAZ)
 2500 CONTINUE
      DO 15 K=2,N1Y
```

```
      DO 15 I=2,N1Y
      AKY(K,I)=(-BY(K,1)*A1Y(I)/AY(1,1)+BY(K,I)+
     1BY(K,NTY)*A2Y(I)/DENY)
      AVY(K,I)=(-AY(K,1)*A1Y(I)/AY(1,1)+AY(K,I)+
     1AY(K,NTY)*A2Y(I)/DENY)
   15 CONTINUE
      DO 155 L=2,N1Z
      DO 155 I=2,N1Z
      AKZ(L,I)=(-BZ(L,1)*A1Z(I)/AZ(1,1)+BZ(L,I)+
     1BZ(L,NTZ)*A2Z(I)/DENZ)
      DAKZ(L,I)=(-AZ(L,1)*A1Z(I)/AZ(1,1)+AZ(L,I)+
     1AZ(L,NTZ)*A2Z(I)/DENZ)
  155 CONTINUE
      DO 10 J=1,NS
      DO 10 I=1,NS
   10 PW(J,I)=0.D0
      DO 113 K=1,NZ
      DO 113 IJ=1,NY
      JJ=IJ+(K-1)*NY
      DO 112 J=1,NZ
      I=IJ+(J-1)*NY
  112 PW(JJ,I)=PW(JJ,I)+AKZ(K+1,J+1)*R6(K+1)/R1(K+1)+
     1DAKZ(K+1,J+1)*R3(K+1)/R1(K+1)
      DO 14 J=1,NY
      I=J+(K-1)*NY
   14 PW(JJ,I)=PW(JJ,I)+AKY(IJ+1,J+1)*R5(K+1)/R1(K+1)-
     1AVY(IJ+1,J+1)*R2(K+1)/R1(K+1)
  113 CONTINUE
C
C     INTEGRATION USING DRKGS
C
    1 CONTINUE
      SUM=0.D0
      KK=NDIM-1
      DO 31 I=1,KK
      PY(I)=1.D0/DFLOAT(NDIM)
```

```
   31 SUM=SUM+DY(I)
      DY(NDIM)=1.D0-SUM
      X0=PRMT(1)
      DX0=DX
      PRMT(2)=PRMT(1)+DX
      PRMT(3)=DX
      CALL DRKGS(PRMT,P,DY,NDIM,IHLF,FCT,AUX,PW)
      X=PRMT(1)
   65 IF(X.GT.1.00D0) STOP
      IF(X.GE..99D-07) DX=3.0D-07
      IF(X.GE..99D-06) DX=3.0D-06
      IF(X.GE..99D-05) DX=1.0D-05
      IF(X.GE..99D-04) DX=0.5D-04
      IF(X.GE..99D-03) DX=0.25D-03
      IF(X.GE..99D-02) DX=0.25D-02
      IF(X.GE..99D-01) DX=0.10D-01
      IF(X.GE..499) DX=0.25D-01
      IF(X.GT.0.1D-01) IICKY=1
C
C     TRANSFORMATION OF THE DRKGS RESULTS INTO A C(Y,Z) FORM
C
      J=1
      L1=1
      L2=NY
   81 DO 70 L=L1,L2
      K=L-(J-1)*NY
      KK=K+1
      JJ=J+1
      C(KK,JJ)=P(L)
   70 CONTINUE
      J=J+1
      IF(J.GT.NZ) GO TO 82
      L1=L2+1
      L2=L2+NY
      GO TO 81
   82 CONTINUE
```

```
C                                                                    MAIN2880
C      CALCULATION OF THE BOUNDARY CONCENTRATIONS                    MAIN2890
C                                                                    MAIN2900
       DO 83 I=1,NTZ                                                 MAIN2910
       C(1,I)=0.0D0                                                  MAIN2920
    83 C(NTY,I)=0.0D0                                                MAIN2930
       DO 833 J=1,NTY                                                MAIN2940
       C(J,1)=0.0D0                                                  MAIN2950
   833 C(J,NTZ)=0.0D0                                                MAIN2960
       DO 84 L=2,N1Z                                                 MAIN2970
       DO 84 I=2,N1Y                                                 MAIN2980
       C(1,L)=C(1,L)-A1Y(I)*C(I,L)/AY(1,1)                           MAIN2990
    84 C(NTY,L)=C(NTY,L)+A2Y(I)*C(I,L)/DENY                          MAIN3000
       DO 844 K=2,N1Y                                                MAIN3010
       DO 844 I=2,N1Z                                                MAIN3020
       C(K,1)=C(K,1)-A1Z(I)*C(K,I)/AZ(1,1)                           MAIN3030
   844 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/DENZ                          MAIN3040
       DO 85 I=2,N1Y                                                 MAIN3050
       C(1,1)=C(1,1)-A1Y(I)*C(I,1)/AY(1,1)                           MAIN3060
       C(NTY,1)=C(NTY,1)+A2Y(I)*C(I,1)/DENY                          MAIN3070
       C(1,NTZ)=C(1,NTZ)-A1Y(I)*C(I,NTZ)/AY(1,1)                     MAIN3080
    85 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY                    MAIN3090
C                                                                    MAIN3100
C      CALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATION    MAIN3110
C                                                                    MAIN3120
       CALL INTRP(12,NTZ,RSEL,RTZ,FAZ,ZINTP)                         MAIN3130
       DO 855 J=1,NTY                                                MAIN3140
       EHCO(J)=0.D0                                                  MAIN3150
       DO 855 I=1,NTZ                                                MAIN3160
   855 EHCO(J)=EHCO(J)+ZINTP(I)*C(J,I)                               MAIN3170
C                                                                    MAIN3180
C      CALCULATION OF THE CONCENTRATIONS AT Y=0                      MAIN3190
C                                                                    MAIN3200
       CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)                          MAIN3210
       DO 856 J=1,NTZ                                                MAIN3220
       CECO(J)=0.D0                                                  MAIN3230
```

```
      DO 856 I=1,NTY                                                    MAIN3240
  856 CECO(J)=CECO(J)+YINTP(I)*C(I,J)                                   MAIN3250
      CCO1=0.D0                                                         MAIN3260
      CCO2=0.D0                                                         MAIN3270
      CCO3=0.D0                                                         MAIN3280
      DO 857 I=1,NTY                                                    MAIN3290
      CCO1=CCO1+YINTP(I)*EHCO(I)                                        MAIN3300
  857 CONTINUE                                                          MAIN3310
      COY=EHCO(1)                                                       MAIN3320
      C1Y=EHCO(NTY)                                                     MAIN3330
C                                                                       MAIN3340
C     CALCULATION OF THE MASS RATE                                      MAIN3350
C                                                                       MAIN3360
      Q=0.0D0                                                           MAIN3370
      DO 47 I=2,N1Y                                                     MAIN3380
      DO 47 J=2,N1Z                                                     MAIN3390
   47 Q=Q+WY(I)*WZ(J)*C(I,J)*U(J)                                       MAIN3400
      Q=2.D0*YMAX*(D1Y+D2Y+2.D0*BETAY)*H*(D1Z+D2Z+2.D0*BETAZ)*Q         MAIN3410
      Q=1000.D0/60.D0*Q                                                 MAIN3420
      ACTX=X*XMAX                                                       MAIN3430
C                                                                       MAIN3440
C     CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS                 MAIN3450
C                                                                       MAIN3460
      RYC=(BETAY+D1Y+PV*ACTX/2.D0/YMAX)/(D1Y+D2Y+2.D0*BETAY)            MAIN3470
      DO 859 J=1,NTZ                                                    MAIN3480
  859 CECOY(J)=0.D0                                                     MAIN3490
      IF(RYC.GE.1.0D0) IST=1                                            MAIN3500
      CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)                              MAIN3510
      DO 860 J=1,NTZ                                                    MAIN3520
      DO 860 I=1,NTY                                                    MAIN3530
  860 CECOY(J)=CECOY(J)+YINTP(I)*C(I,J)                                 MAIN3540
      ARYC=PV*ACTX                                                      MAIN3550
      DO 858 I=1,NTZ                                                    MAIN3560
      CCO2=CCO2+ZINTP(I)*CECO(I)                                        MAIN3570
      CCO3=CCO3+ZINTP(I)*CECOY(I)                                       MAIN3580
  858 CONTINUE                                                          MAIN3590
```

```
      C0Z=CECOY(1)
      C1Z=CECOY(NTZ)
      EPS=CC03*RATIO
C
C     TEST FOR THE PLUME SPREAD BY COMPARISON OF BOUNDARY
C     CONCENTRATIONS WITH EPS (= C(TRUE CENTERLINE,EFFECTIVE
C     EMISSION HEIGHT)*RATIO)
C       - IF OK, PRINT RESULTS AND ADVANCE INTEGRATION (12)
C       - IF NOT, GET NEW INITIAL CONDITION AND INTEGRATE AGAIN
C
      IF(IOKYP.EQ.2.AND.IOKYM.EQ.2) GO TO 12
      IOKY=0
      IOKZ=0
      IF((C0Y).LT.EPS.AND.(C1Y).LT.EPS) IOKY=1
      IF(VAR1Y.LT.1.0D-08.AND.VAR2Y.LT.1.0D-08) IOKY=1
      IF(VAR1Y.LT.1.0D-08.AND.(C1Y).LT.EPS) IOKY=1
      IF(VAR2Y.LT.1.0D-08.AND.(C0Y).LT.EPS) IOKY=1
      IF(IOKY.EQ.1) GO TO 13
      IF(D1Y.LT.0.5D0-BETAY-1.0D-08.AND.(C0Y).GT.EPS)D1Y=D1Y+
     1DD1Y*DMULY
      IF(VAR2Y.GT.1.0D-08.AND.(C1Y).GT.EPS) D2Y=D2Y+DD2Y*DMULY
      IOKY=0
      IF(IOKYP.EQ.1) IOKYP=2
      IF(IOKYP.EQ.0) IOKYP=1
   13 CONTINUE
      IF(IIOKY.EQ.0) GO TO 1333
      IF(C0Y.GT.0.D0.AND.C1Y.GT.0.D0) GO TO 1333
      IF((C0Y).LT.0.0D0)D1Y=D1Y-DD1Y*DMULY/2.5D0
      IF((C1Y).LT.0.0D0) D2Y=D2Y-DD2Y*DMULY/2.5D0
      IOKY=0
      IF(IOKYM.EQ.1) IOKYM=2
      IF(IOKYM.EQ.0) IOKYM=1
 1333 CONTINUE
      IF((C0Z).LT.EPS.AND.(C1Z).LT.EPS) IOKZ=1
      IF(VAR1Z.LT.1.0D-08.AND.VAR2Z.LT.1.0D-08) IOKZ=1
      IF(VAR1Z.LT.1.0D-08.AND.(C1Z).LT.EPS) IOKZ=1
```

```
      IF(VAR2Z.LT.1.0D-08.AND.(C0Z).LT.EPS) ICKZ=1                      MAIN3960
      IF(ICKY.EQ.1.AND.IOKZ.EQ.1) GO TO 12                              MAIN3970
      IF(D1Z.LT.SEL-BETAZ-1.0D-08.AND.(C0Z).GT.EPS)D1Z=D1Z+             MAIN3980
     1DD1Z*DMULZ                                                        MAIN3990
      IF(VAR2Z.GT.1.0D-08.AND.(C1Z).GT.EPS) D2Z=D2Z+DD2Z*DMULZ          MAIN4000
      IOKZ=1                                                            MAIN4010
  133 CONTINUE                                                          MAIN4020
      IF(IOKY.EQ.1.AND.IOKZ.EQ.1) GO TO 12                              MAIN4030
      IF(X.GE..99D-03) DMULY=2.D0                                       MAIN4040
      IF(X.GE..99D-02) DMULY=6.D0                                       MAIN4050
      IF(X.GE..99D-01) DMULY=10.D0                                      MAIN4060
      IF(X.GE..99D-03) DMULZ=4.D0                                       MAIN4070
      IF(X.GE..99D-02) DMULZ=12.D0                                      MAIN4080
      IF(X.GE..99D-01) DMULZ=16.D0                                      MAIN4090
      IF(0.5D0-BETAY-D1Y.LE.DD1Y*DMULY) DD1Y=(0.5D0-BETAY-D1Y)/DMULY    MAIN4100
      IF(1.D0-0.5D0-BETAY-D2Y.LE.DD2Y*DMULY)DD2Y=(1.D0-0.5D0-BETAY-D2Y)/MAIN4110
     1DMULY                                                             MAIN4120
      IF(SEL-BETAZ-D1Z.LE.DD1Z*DMULZ) DD1Z=(SEL-BETAZ-D1Z)/DMULZ        MAIN4130
      IF(1.D0-SEL-BETAZ-D2Z.LE.DD2Z*DMULZ)DD2Z=(1.D0-SEL-BETAZ-D2Z)/    MAIN4140
     1DMULZ                                                             MAIN4150
C                                                                       MAIN4160
C     CALCULATION OF NEW INITIAL CONDITION                              MAIN4170
C                                                                       MAIN4180
      X=X0                                                              MAIN4190
      PRMT(1)=X0                                                        MAIN4200
      DX=DX0                                                            MAIN4210
      NCI=1                                                             MAIN4220
   96 DO 92 I=1,NY                                                      MAIN4230
      J=I+1                                                             MAIN4240
      VIY=((D1Y+D2Y+2.D0*BETAY)*RTY(I+1)+D10Y-D1Y)/(D10Y+D20Y+          MAIN4250
     12.D0*BETAY)                                                       MAIN4260
      IF(VIY.LT.1.0D0) GO TO 90                                         MAIN4270
      C(J,NCI)=0.0D0                                                    MAIN4280
      GO TO 92                                                          MAIN4290
   90 IF(VIY.GT.0.0D0) GO TO 95                                         MAIN4300
      C(J,NCI)=0.0D0                                                    MAIN4310
```

```
      GO TO 92
   95 CALL INTRP(12,NTY,VIY,RTY,FAY,YINTP)
      C(J,NCI)=CC(1,NCI)*YINTP(1)+CC(NTY,NCI)*YINTP(NTY)
      DO 93 K=1,NY
   93 C(J,NCI)=C(J,NCI)+YINTP(K+1)*CC(K+1,NCI)
   92 CONTINUE
      NCI=NCI+1
      IF(NCI.GT.NTZ) GO TO 955
      GO TO 96
  955 NCI=1
 1000 DO 42 I=1,NZ
      J=NCI+(I-1)*NY
      VIZ=((D1Z+D2Z+2.D0*BETAZ)*RTZ(I+1)+D10Z-D1Z)/(D10Z+D20Z+
     12.0D0*BETAZ)
      IF(VIZ.LT.1.0D0) GO TO 40
      P(J)=0.0D0
      GO TO 42
   40 IF(VIZ.GT.0.0D0) GO TO 45
      P(J)=0.0D0
      GO TO 42
   45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP)
      P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ)
      DO 43 K=1,NZ
   43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1)
   42 CONTINUE
      NCI=NCI+1
      IF(NCI.GT.NY) GO TO 20
      GO TO 1000
C
C     PRINT AND STORE THE RESULTS
C
   12 CONTINUE
      IOKYP=0
      IOKYM=0
      D10Y=D1Y
      D20Y=D2Y
```

```
      D10Z=D1Z                                                          MAIN4680
      D20Z=D2Z                                                          MAIN4690
      DO 66 I=1,NTY                                                     MAIN4700
      EHCO(I)=1000.D0*EHCO(I)                                           MAIN4710
      DO 66 J=1,NTZ                                                     MAIN4720
      IF(I.EQ.1) CECO(J)=CECO(J)*1000.D0                                MAIN4730
      IF(I.EQ.1) CECOY(J)=CECOY(J)*1000.D0                              MAIN4740
      CC(I,J)=C(I,J)                                                    MAIN4750
   66 C(I,J)=C(I,J)*1000.D0                                             MAIN4760
      CC01=1000.D0*CC01                                                 MAIN4770
      CC03=1000.D0*CC03                                                 MAIN4780
      WRITE(6,500) ACTX,Q,IHLF                                          MAIN4790
  500 FORMAT(2(/),20X,'X =',F12.3,20X,'Q =',F10.2,10X,'IHLF =',I5,/)    MAIN4800
      WRITE(6,2000)                                                     MAIN4810
 2000 FORMAT(2(/))                                                      MAIN4820
      WRITE(6,352) (ACTY(I),I=1,NTYH),ARYC                              MAIN4830
  352 FORMAT(1X,132('*')/1X,'*    Z/Y   *',10F12.2,'    *')             MAIN4840
      WRITE(6,650)                                                      MAIN4850
   68 CONTINUE                                                          MAIN4860
      I=NTZ                                                             MAIN4870
  502 CONTINUE                                                          MAIN4880
      WRITE(6,300) ACTZ(I),(C(J,I),J=1,NTYH),CECO(I)                    MAIN4890
  300 FORMAT(1X,'*',F7.2,1X,'*',10F12.5,'    *')                        MAIN4900
      I=I-1                                                             MAIN4910
      IF(I.EQ.0) GO TO 501                                              MAIN4920
      GO TO 502                                                         MAIN4930
  501 CONTINUE                                                          MAIN4940
      WRITE(6,650)                                                      MAIN4950
  650 FORMAT(1X,132('*'))                                               MAIN4960
      WRITE(6,300) HSEL,(EHCO(I),I=1,NTYH),CC01                         MAIN4970
      WRITE(6,2000)                                                     MAIN4980
      WRITE(6,352) (ACTY(I),I=NTYH1,NTY),ARYC                           MAIN4990
      WRITE(6,650)                                                      MAIN5000
  668 CONTINUE                                                          MAIN5010
      I=NTZ                                                             MAIN5020
 5502 CONTINUE                                                          MAIN5030
```

```
      WRITE(6,300) ACTZ(I),(C(J,I),J=NTYH1,NTY),CECOY(I)             MAIN5040
      I=I-1                                                          MAIN5050
      IF(I.EQ.0) GO TO 5501                                          MAIN5060
      GO TO 5502                                                     MAIN5070
 5501 CONTINUE                                                       MAIN5080
      WRITE(6,650)                                                   MAIN5090
      WRITE(6,300) HSEL,(EHCC(I),I=NTYH1,NTY),CCC3                   MAIN5100
      IF(IST.EQ.1) STOP                                              MAIN5110
      GO TO 1                                                        MAIN5120
  900 CONTINUE                                                       MAIN5130
      END                                                            MAIN5140
```

```
      SUBROUTINE DRKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,AUX,PW)               DRKG  10
C                                                                       DRKG  20
C                                                                       DRKG  30
C   THIS SUBROUTINE SOLVES A SYSTEM OF FIRST ORDER ORDINARY DIFFERENTIAL DRKG  40
C   EQUATIONS WITH GIVEN INITIAL CONDITIONS                             DRKG  50
C                                                                       DRKG  60
C                                                                       DRKG  70
C      PRMT        - AN INPUT OUTPUT VECTOR WITH DIMENSION GREATER OR   DRKG  80
C                    EQUAL TO 5                                         DRKG  90
C      PRMT(1)     - LOWER BOUND OF THE INTERVAL                        DRKG 100
C      PRMT(2)     - UPPER BOUND OF THE INTERVAL                        DRKG 110
C      PRMT(3)     - INITIAL INCREMENT OF THE INDEPENDENT VARIABLE      DRKG 120
C      PRMT(4)     - UPPER ERROR BOUND                                  DRKG 130
C      PRMT(5)     - NO INPUT PARAMETER. IT IS 0 UNLESS THE USER WANTS TO DRKG 140
C                    TERMINATE RKGS AT ANY OUTPUT POINT                 DRKG 150
C      DERY        - INPUT VECTOR OF ERROR WEIGHTS. LATERON IS THE VECTOR DRKG 160
C                    OF DERIVATIVES                                     DRKG 170
C      NDIM        - THE NUMBER OF EQUATIONS IN THE SYSTEM              DRKG 180
C      IHLF        - THE NUMBER OF BISECTIONS OF THE INITIAL INCREMENT  DRKG 190
C      AUX         - AN AUXILIARY STORAGE ARRAY (8 ROWS AND NDIM COLUMNS) DRKG 200
C                                                                       DRKG 210
C                                                                       DRKG 220
      IMPLICIT REAL*8(A-H,O-Z)                                          DRKG 230
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(1),           DRKG 240
     1PW(NDIM,NDIM)                                                     DRKG 250
      DO 1 I=1,NDIM                                                     DRKG 260
    1 AUX(8,I)=DERY(I)/15.D0                                            DRKG 270
      X=PRMT(1)                                                         DRKG 280
      XEND=PRMT(2)                                                      DRKG 290
      H=PRMT(3)                                                         DRKG 300
      PRMT(5)=0.D0                                                      DRKG 310
      CALL FCT(Y,NDIM,DERY,PW)                                          DRKG 320
C                                                                       DRKG 330
C   ERROR TEST                                                          DRKG 340
C                                                                       DRKG 350
```

```
      IF(H*(XEND-X))36,37,2                                              DRKG 360
C                                                                        DRKG 370
C     PREPARATIONS FOR RUNGE-KUTTA METHOD                                DRKG 380
C                                                                        DRKG 390
    2 A(1)=.5D0                                                          DRKG 400
      A(2)=.29289321881345248D0                                          DRKG 410
      A(3)=1.7071067811865475D0                                          DRKG 420
      A(4)=.16666666666666667D0                                          DRKG 430
      B(1)=2.D0                                                          DRKG 440
      B(2)=1.D0                                                          DRKG 450
      B(3)=1.D0                                                          DRKG 460
      B(4)=2.D0                                                          DRKG 470
      C(1)=.5D0                                                          DRKG 480
      C(2)=.29289321881345248D0                                          DRKG 490
      C(3)=1.7071067811865475D0                                          DRKG 500
      C(4)=.5D0                                                          DRKG 510
C                                                                        DRKG 520
C     PREPARATIONS OF FIRST RUNGE-KUTTA STEP                             DRKG 530
C                                                                        DRKG 540
      DO 3 I=1,NDIM                                                      DRKG 550
      AUX(1,I)=Y(I)                                                      DRKG 560
      AUX(2,I)=DERY(I)                                                   DRKG 570
      AUX(3,I)=0.D0                                                      DRKG 580
    3 AUX(6,I)=0.D0                                                      DRKG 590
      IREC=0                                                             DRKG 600
      H=H+H                                                              DRKG 610
      IHLF=-1                                                            DRKG 620
      ISTEP=0                                                            DRKG 630
      IEND=0                                                             DRKG 640
C                                                                        DRKG 650
C     START OF A RUNGE-KUTTA STEP                                        DRKG 660
C                                                                        DRKG 670
    4 IF((X+H-XEND)*H)7,6,5                                              DRKG 680
    5 H=XEND-X                                                           DRKG 690
    6 IEND=1                                                             DRKG 700
C                                                                        DRKG 710
```

```
      C   RECORDING OF INITIAL VALUES OF THIS STEP                      DRKG 720
      C                                                                 DRKG 730
          7 CONTINUE                                                    DRKG 740
            IF(PRMT(5))40,8,40                                          DRKG 750
          8 ITEST=0                                                     DRKG 760
          9 ISTEP=ISTEP+1                                               DRKG 770
      C                                                                 DRKG 780
      C   START OF INNERMOST RUNGE-KUTTA LOOP                           DRKG 790
      C                                                                 DRKG 800
            J=1                                                         DRKG 810
         10 AJ=A(J)                                                     DRKG 820
            BJ=B(J)                                                     DRKG 830
            CJ=C(J)                                                     DRKG 840
            DO 11 I=1,NDIM                                              DRKG 850
            R1=H*DERY(I)                                                DRKG 860
            R2=AJ*(R1-BJ*AUX(6,I))                                      DRKG 870
            Y(I)=Y(I)+R2                                                DRKG 880
            R2=R2+R2+R2                                                 DRKG 890
         11 AUX(6,I)=AUX(6,I)+R2-CJ*R1                                  DRKG 900
            IF(J-4)12,15,15                                             DRKG 910
         12 J=J+1                                                       DRKG 920
            IF(J-3)13,14,13                                             DRKG 930
         13 X=X+.5D0*H                                                  DRKG 940
         14 CALL FCT(Y,NDIM,DERY,PW)                                    DRKG 950
            GOTO 10                                                     DRKG 960
      C                                                                 DRKG 970
      C   TEST OF ACCURACY                                              DRKG 980
      C                                                                 DRKG 990
         15 IF(ITEST)16,16,20                                           DRKG1000
      C                                                                 DRKG1010
      C   IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING OF ACCURACY DRKG1020
      C                                                                 DRKG1030
         16 DO 17 I=1,NDIM                                              DRKG1040
         17 AUX(4,I)=Y(I)                                               DRKG1050
            ITEST=1                                                     DRKG1060
            ISTEP=ISTEP+ISTEP-2                                         DRKG1070
```

```
   18 IHLF=IHLF+1                                                       DRKG1080
      X=X-H                                                             DRKG1090
      H=.5D0*H                                                          DRKG1100
      DO 19 I=1,NDIM                                                    DRKG1110
      Y(I)=AUX(1,I)                                                     DRKG1120
      DERY(I)=AUX(2,I)                                                  DRKG1130
   19 AUX(6,I)=AUX(3,I)                                                 DRKG1140
      GOTO 9                                                            DRKG1150
C                                                                       DRKG1160
C  IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE                      DRKG1170
C                                                                       DRKG1180
   20 IMOD=ISTEP/2                                                      DRKG1190
      IF(ISTEP-IMOD-IMOD)21,23,21                                       DRKG1200
   21 CALL FCT(Y,NDIM,DERY,PW)                                          DRKG1210
      DO 22 I=1,NDIM                                                    DRKG1220
      AUX(5,I)=Y(I)                                                     DRKG1230
   22 AUX(7,I)=DERY(I)                                                  DRKG1240
      GOTO 9                                                            DRKG1250
C                                                                       DRKG1260
C  COMPUTATION OF TEST VALUE DELT                                       DRKG1270
C                                                                       DRKG1280
   23 DELT=0.D0                                                         DRKG1290
      DO 24 I=1,NDIM                                                    DRKG1300
   24 DELT=DELT+AUX(8,I)*DABS(AUX(4,I)-Y(I))                            DRKG1310
      IF(DELT-PRMT(4))28,28,25                                          DRKG1320
C                                                                       DRKG1330
C  ERROR IS TOO GREAT                                                   DRKG1340
C                                                                       DRKG1350
   25 IF(IHLF-10)26,36,36                                               DRKG1360
   26 DO 27 I=1,NDIM                                                    DRKG1370
   27 AUX(4,I)=AUX(5,I)                                                 DRKG1380
      ISTEP=ISTEP+ISTEP-4                                               DRKG1390
      X=X-H                                                             DRKG1400
      IEND=0                                                            DRKG1410
      GOTO 18                                                           DRKG1420
C                                                                       DRKG1430
```

```
      C   RESULT VALUES ARE GOOD                                              DRKG1440
      C                                                                       DRKG1450
         28 CALL FCT(Y,NDIM,DERY,PW)                                          DRKG1460
            DO 29 I=1,NDIM                                                    DRKG1470
            AUX(1,I)=Y(I)                                                     DRKG1480
            AUX(2,I)=DERY(I)                                                  DRKG1490
            AUX(3,I)=AUX(6,I)                                                 DRKG1500
            Y(I)=AUX(5,I)                                                     DRKG1510
         29 DERY(I)=AUX(7,I)                                                  DRKG1520
            IF(PRMT(5))40,30,40                                               DRKG1530
         30 DO 31 I=1,NDIM                                                    DRKG1540
            Y(I)=AUX(1,I)                                                     DRKG1550
         31 DERY(I)=AUX(2,I)                                                  DRKG1560
            IREC=IHLF                                                         DRKG1570
            IF(IEND)32,32,39                                                  DRKG1580
      C                                                                       DRKG1590
      C   INCREMENT GETS DOUBLED                                              DRKG1600
      C                                                                       DRKG1610
         32 IHLF=IHLF-1                                                       DRKG1620
            ISTEP=ISTEP/2                                                     DRKG1630
            H=H+H                                                             DRKG1640
            IF(IHLF)4,33,33                                                   DRKG1650
         33 IMOD=ISTEP/2                                                      DRKG1660
            IF(ISTEP-IMOD-IMOD)4,34,4                                         DRKG1670
         34 IF(DELT-.02D0*PRMT(4))35,35,4                                     DRKG1680
         35 IHLF=IHLF-1                                                       DRKG1690
            ISTEP=ISTEP/2                                                     DRKG1700
            H=H+H                                                             DRKG1710
            GOTO 4                                                            DRKG1720
      C                                                                       DRKG1730
      C   RETURNS TO CALLING PROGRAM                                          DRKG1740
      C                                                                       DRKG1750
         36 IHLF=11                                                           DRKG1760
            CALL FCT(Y,NDIM,DERY,PW)                                          DRKG1770
            GOTO 39                                                           DRKG1780
         37 IHLF=12                                                           DRKG1790
```

```
      GOTO 39                                                          DRKG1800
   38 IHLF=13                                                          DRKG1810
   39 CONTINUE                                                         DRKG1820
      PRMT(1)=X                                                        DRKG1830
   50 FORMAT(2(/),20X,'X =',F16.12,10X,'IHLF =',I5)                    DRKG1840
   40 RETURN                                                           DRKG1850
      END                                                              DRKG1860
```

```
      SUBROUTINE FCT(YP,M,DY,PW)                                    FCT   10
C                                                                   FCT   20
C                                                                   FCT   30
C     THIS SUBROUTINE COMPUTES THE DERIVATIVES (RIGHT HAND SIDES)   FCT   40
C     OF THE SYSTEM TO GIVEN VALUES OF YP(CONCENTRATION)            FCT   50
C                                                                   FCT   60
C                                                                   FCT   70
      IMPLICIT REAL*8(A-H,O-Z)                                      FCT   80
      DIMENSION YP(M),DY(M),PW(M,M)                                 FCT   90
      DO 15 J=1,M                                                   FCT  100
      DY(J)=0.0D0                                                   FCT  110
      DO 10 I=1,M                                                   FCT  120
   10 DY(J)=DY(J)+PW(J,I)*YP(I)                                     FCT  130
   15 CONTINUE                                                      FCT  140
      RETURN                                                        FCT  150
      END                                                           FCT  160
```

```
      SUBROUTINE VELDIF(XZ,H,UGR,UST,AM,U,V,ISTB,ALPHA,N3,AKY,AKZ,DAKZ,   VELD  10
     1SEL,IND,US,DKN,DUN,HSKN,HGEO,AMM)                                   VELD  20
C                                                                         VELD  30
C                                                                         VELD  40
C     THIS SUBROUTINE CALCULATES THE VELOCITY AND TURBULENT               VELD  50
C     DIFFUSIVITY VECTORS (TWO-DIMENSIONS) AS FUNCTIONS OF                VELD  60
C     ELEVATION AND STABILITY CLASS                                       VELD  70
C                                                                         VELD  80
C                                                                         VELD  90
      IMPLICIT REAL*8(A-H,O-Z)                                            VELD 100
      DIMENSION XZ(12),AKY(12),AKZ(12),DAKZ(12),COEFK(6),DKN(6),          VELD 110
     1TDFKN(6),DUN(6),TDFUN(6),U(12),V(12),HGEO(6)                        VELD 120
      DATA COEFK/570.D0,555.D0,540.D0,222.D0,0.D0,-70.5D0/                VELD 130
      IF(IND.NE.0) GO TO 5                                                VELD 140
      US=UST*(1.D0-DEXP(-SEL*H/AM)*DCOS(SEL*H/AM))                        VELD 150
      RETURN                                                              VELD 160
    5 CONTINUE                                                            VELD 170
      TDFKN(ISTB)=DKN(ISTB)/H                                             VELD 180
      U(1)=UGR                                                            VELD 190
      PV=DEXP(-DKN(ISTB)/AM)*DSIN(DKN(ISTB)/AM)/                          VELD 200
     1(1.D0-DEXP(-DKN(ISTB)/AM)*DCOS(DKN(ISTB)/AM))                       VELD 210
      U1=UST*(1.D0-DEXP(-DKN(ISTB)/AM)*DCOS(DKN(ISTB)/AM))/               VELD 220
     1(DKN(ISTB)/DUN(ISTB))**AMM                                          VELD 230
      V(1)=-PV*U(1)                                                       VELD 240
      TDFUN(ISTB)=HGEO(ISTB)/H                                            VELD 250
      DO 25 L=2,N3                                                        VELD 260
      U(L)=UST*(1.D0-DEXP(-XZ(L)*H/AM)*DCOS(XZ(L)*H/AM))                  VELD 270
      IF(XZ(L).LE.TDFKN(ISTB)) U(L)=U1*(XZ(L)*H/DUN(ISTB))**AMM           VELD 280
      IF(XZ(L).LT.TDFUN(ISTB)) V(L)=-UST*DEXP(-XZ(L)*H/AM)*               VELD 290
     1DSIN(XZ(L)*H/AM)                                                    VELD 300
      IF(XZ(L).GE.TDFUN(ISTB)) V(L)=0.D0                                  VELD 310
      IF(XZ(L).LT.TDFKN(ISTB)) V(L)=-PV*U(L)                              VELD 320
   25 CONTINUE                                                            VELD 330
      IF(ISTB.GE.5) GO TO 10                                              VELD 340
      IF(DKN(ISTB).GT.1.D-08) GO TO 20                                    VELD 350
```

```
      DO 4 L=2,N3                                                       VELD 360
      AKZ(L)=COEFK(ISTB)+90.D0                                          VELD 370
      DAKZ(L)=0.D0                                                      VELD 380
    4 AKY(L)=ALPHA*AKZ(L)                                               VELD 390
      RETURN                                                            VELD 400
   20 CONTINUE                                                          VELD 410
      TDSKN=1.D0-100.D0/H                                               VELD 420
      IF(H.LE.HSKN) TDSKN=1.D0                                          VELD 430
      DO 2 L=2,N3                                                       VELD 440
      IF(XZ(L)-TDFKN(ISTB)) 11,12,12                                    VELD 450
   11 AKZ(L)=COEFK(ISTB)*XZ(L)/TDFKN(ISTB)+90.D0                        VELD 460
      DAKZ(L)=COEFK(ISTB)/DKN(ISTB)                                     VELD 470
      GO TO 16                                                          VELD 480
   12 IF(XZ(L)-TDSKN) 13,13,14                                          VELD 490
   13 AKZ(L)=COEFK(ISTB)+90.D0                                          VELD 500
      DAKZ(L)=0.D0                                                      VELD 510
      GO TO 15                                                          VELD 520
   14 AKZ(L)=COEFK(ISTB)*H*(1.D0-XZ(L))/100.D0+90.D0                    VELD 530
      DAKZ(L)=-COEFK(ISTB)/100.D0                                       VELD 540
   15 CONTINUE                                                          VELD 550
   16 AKY(L)=ALPHA*(COEFK(ISTB)+90.D0)                                  VELD 560
    2 CONTINUE                                                          VELD 570
      GO TO 50                                                          VELD 580
   10 CONTINUE                                                          VELD 590
      DO 3 L=2,N3                                                       VELD 600
      AKZ(L)=COEFK(ISTB)+90.D0                                          VELD 610
      DAKZ(L)=0.D0                                                      VELD 620
    3 AKY(L)=ALPHA*AKZ(L)                                               VELD 630
   50 CONTINUE                                                          VELD 640
      RETURN                                                            VELD 650
      END                                                               VELD 660
```

```
C
C
C      INPUT DATA REQUIRED
C
C
   10   10    4
     4000.0D+00      500.0D+00     4000.0D+00     8.9000D+00        0.0
     687.22D+00      322.49D+00      30.0D+00     60.0000D+00        0.20
  50.0D+00  50.0D+00  50.0D+00  50.0D+00  50.0D+00  50.0D+00
  10.0D+00  10.0D+00  10.0D+00  10.0D+00  10.0D+00  10.0D+00
147.35D+01145.67D+01143.97D+01101.31D+01544.14D+00253.28D+00
          .0D+00        0.1D-06        0.1D-06     1.0000D-07
     .2861D-02      .2861D-02        0.1D-01     0.012D-01
     .2861D-02      .2861D-02       0.12D-02
       0.0D+00        0.1D-06       0.25D-02       0.25D-02
     .2500D-02      .2500D-02     1500.0D+00       0.14D+00
```

APPENDIX B

NOMENCLATURE

a	Constant in equation (3.14)
A_{ij}	Element of the discretizational matrix of first derivatives
B_{ij}	Element of the discretizational matrix of second derivatives
C	Mean concentration, mg/m^3
C_a	Mean concentration obtained by an analytical solution
C_c	Mean concentration calculated by the present work
C_i	Mean concentration at the i-th interior orthogonal collocation point - two-dimensional models
C_o	Equivalent mean concentration at the source
$C_{k\ell}$	Mean concentration at the interior orthogonal collocation point (η_k, ζ_ℓ) - three-dimensional models
e	Absolute error defined by equation (3.1), %
E_{ij}	Elements of the collocation matrix
f	Coriolis parameter, sec^{-1}
H	Effective emission height, m
k_1	Reaction rate constant, min^{-1}
K	Turbulent diffusivity, m^2/sec
K_1	Turbulent diffusivity at an elevation z_1
m	Exponent in power-law form for the mean wind velocity profile
n	Exponent in power-law form for the turbulent diffusivity profile
N	Number of interior orthogonal collocation points.

p	Atmospheric pressure
Q	Source strength, kg/sec unless otherwise specified
Q_x	Mass rate through y-z plane at x=constant, gm/sec unless otherwise specified
r	Parameter in equation (2.9)
r	Mathematical parameter that represents the ratio of boundary to centerline concentration
R	Rate of generation of species
s	Parameter in equation (2.9)
t	Time, sec
u	Mean wind velocity in the x-direction, m/sec unless otherwise specified
u_1	Mean wind velocity at an elevation z_1
u_{10}	Mean wind velocity at 10 meters
$\underline{\underline{U}}$	Eigenvectors of matrix E
$\underline{\underline{U}}^{-1}$	Eigenrows of matrix E
v	Mean wind velocity in the y-direction, m/sec unless otherwise specified
w	Mean wind velocity in the z-direction, m/sec unless otherwise specified
W	Quadrature weights
x	Cartesian coordinate in mean wind direction, m unless otherwise specified
x_{max}	Maximum distance in the x-direction, m
y	Cartesian coordinate in lateral direction, m
y_{max}	Maximum distance in the y-direction, m

z Cartesian coordinate in vertical direction, m

z_{max} Maximum height above terrain (in some cases refers to the elevation of the inversion layer), m

z_1 Reference height, m

Greek Symbols

α Angle between geostrophic velocity and surface boundary layer velocity, °

β Mathematical parameter that represents a source dimension

Γ Gamma function

δ Mathematical parameter used for spatial variable transformations

δ_{ij} Kronecker delta function

Δ Knee height for the vertical turbulent diffusivity profile, m

ε Upper error bound in "DRKGS"

ζ Dimensionless spatial variable in the z-direction

η Dimensionless spatial variable in the y-direction

$\underline{\underline{\Lambda}}$ Eigenvalues of matrix E

ξ Dimensionless spatial variable in the x-direction

ρ Density

σ Standard deviation

τ Eddy stresses

ϕ Geostrophical latitude, °

ψ Variable used in Figure 4.6. Represents ground-level concentration

Superscripts

i	Initial value profile for the concentration
*	Refers to dimensionless spatial variables

Subscripts

G	Refers to geostrophic flow
i	Index in collocation equations
k	Represents the y-direction in collocation equations
ℓ	Represents the z-direction in collocation equations
x	Refers to x coordinate direction
y	Refers to y coordinate direction
z	Refers to z coordinate direction
-	Denotes a vector quantity
=	Refers to a matrix