SOLUTION OF A GENERALIZED AIR POLLUTION MODEL BY ORTHOGONAL COLLOCATION

A Thesis

Presented to

the Faculty of the Department of

Chemical Engineering

The University of Houston

In Partial Fulfillment

of the Requirements for the Degree of

Master of Science in Chemical Engineering

---

by

Miguel T. Fleischer

December, 1975

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Finally, I am glad to dedicate this thesis to my wife, Jackie, and my son, David, whose patience and love have made all of this possible.

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ABSTRACT

Turbulent atmospheric diffusion from single or multiple point sources was simulated using the K-theory and solved by a new numerical technique, orthogonal collocation. The physical and chemical behavior of pollutant species in the atmosphere was described by the 3-dimensional, unsteady-state diffusion equation including chemical reactions. Orthogonal collocation was used to reduce the partial differential equation governing the mean concentration of contaminants to first-order ordinary differential equations. This system of equations was then solved in a digital computer.

Mean wind velocities and turbulent diffusivities were represented by empirical equations. Several meteorological parameters were included in these equations so that a variety of atmospheric conditions can be simulated. These parameters and other information required to solve an air pollution problem must be specified as input data by the user.

The present method was evaluated by comparing the results to existing experimental atmospheric concentration profiles. Good agreement was found in all cases. In addition, the sensitivity of the present model to variations in atmospheric conditions was analyzed by means of a parametric study. Proper responses were observed in all cases.

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CHAPTER I

INTRODUCTION

There has been increasing interest in bringing the air pollution problem under control. This problem can be represented as a system consisting of three basic components: emission sources, the atmosphere, and receptors. Once the pollutants are emitted from sources, they are transported, dispersed, and transformed according to the laws of physics and chemistry throughout the entire atmosphere. Finally, these air pollutants are detected by receptors, such as human beings, animals, plants, and materials, producing in some cases undesirable effects.

In order to understand the cause-effect relationship of pollutant emission and dispersion on the air quality, a study of the three components previously discussed should be carried out. Understanding of the physical and chemical behavior of pollutant species in the atmosphere plays then an important role in the relation of source emissions to air quality standards.

The objective of an air pollution model is to describe mathematically the spatial and temporal history of contaminants released into the atmosphere.

Several air pollution models have been developed so far, but they have had only limited success. An improved dispersion model based on the K-theory and solved using a new numerical technique is presented in this thesis. The atmospheric processes involving air pollutants are described by the 3-dimensional, unsteady-state diffusion equation including chemical reactions. Orthogonal collocation, a weighted residual method, reduces the partial differential equations governing the mean concentration of pollutant species to first-order ordinary differential equations. This system of equations is solved then in a digital computer.

The present work is validated with existing experimental data. In addition, its sensitivity to variations in atmospheric conditions is analyzed by means of a parametric study.

Chapter II

THEORETICAL BACKGROUND

There are two fundamental ways of describing the physical and chemical behavior of pollutant species in the turbulent atmosphere. The first is the so-called Eulerian approach, where the behavior of species is described relative to fixed coordinates. The second is the statistical approach, where concentration changes are described from a statistical point of view by considering the paths of individual elements of fluid, and is thus Lagrangian in nature.

The objective of any air pollution model is to predict pollutant concentrations at given points. These concentrations are caused by emissions from sources, and therefore a source-oriented point of view is the natural one in this case.

Eulerian Approach

Consider s species in a fluid. The concentration of each must, at each instant, satisfy a material balance taken over a volume element. Therefore, the concentration of each species must satisfy the continuity equation usually known as the instantaneous diffusion equation,

$$\frac{\partial C_i}{\partial t} + \frac{\partial}{\partial x_j} u_j C_i = \frac{\partial}{\partial x_j} \{D_i \frac{\partial C_i}{\partial x_j}\} + R_i(C_1,\ldots,C_s) \qquad (2.1)$$

$$i = 1, 2, \ldots, s$$

where the subscript j represents the three coordinate directions: x(axial), y(lateral), and z(vertical); and

C_i = the instantaneous concentration of species i

u_j = the jth component of the fluid velocity

D_i = the molecular diffusivity of species i in the carrier fluid, and

R_i = the rate of generation of species i.

Since atmospheric flows are turbulent, it is conventional to divide the instantaneous quantities into mean and fluctuating facts,

$$C_i = \langle C_i \rangle + C_i' \qquad (2.2)$$

$$u_j = \bar{u}_j + u_j'$$

It should be noted that the mean fluid velocities are usually determined by temporal averaging and the mean concentrations always represent ensemble averages. This is the reason why a different notation has been used for the mean values of the velocities and the concentrations.

Substitution of equation (2.2) into equation (2.1) gives

$$\frac{\partial}{\partial t}(\langle C_i\rangle + C_i') + \frac{\partial}{\partial x_j}\{(\bar{u}_j + u_j')(\langle C_i\rangle + C_i')\} = \frac{\partial}{\partial x_j}\{D_i \frac{\partial}{\partial x_j}(\langle C_i\rangle + C_i')\} + R_i(\langle C_1\rangle + C_1', \ldots, \langle C_s\rangle + C_s') \quad (2.3)$$

Taking an average of equation (2.3) over a large ensemble of realizations of the turbulence, one obtains the following equation governing $\langle C_i\rangle$

$$\frac{\partial\langle C_i\rangle}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_j\langle C_i\rangle) = \frac{\partial}{\partial x_j}\{D_i \frac{\partial\langle C_i\rangle}{\partial x_j} - \langle u_j' C_i'\rangle\} + \langle R_i(\langle C_1\rangle + C_1', \ldots, \langle C_s\rangle + C_s')\rangle \quad (2.4)$$

The most common means of representing the turbulent fluxes $\langle u_j' C_i\rangle$ is by the so-called K-theory, in which a turbulent diffusivity is defined by

$$-\langle u_j' C_i'\rangle = K_{jj} \frac{\partial\langle C_i\rangle}{\partial x_j} \quad (2.5)$$

Ignoring the molecular diffusion when compared with the turbulent diffusion, and assuming the atmosphere to be incompressible, the final expression for the diffusion equation becomes

$$\frac{\partial\langle C_i\rangle}{\partial t} + \bar{u}_j \frac{\partial\langle C_i\rangle}{\partial x_j} = \frac{\partial}{\partial x_j}\{K_{jj} \frac{\partial\langle C_i\rangle}{\partial x_j}\} + \langle R_i(\langle C_1\rangle, \ldots, \langle C_s\rangle)\rangle \quad (2.6)$$

It should be pointed out that the effect of concentration fluctuations on the rate of reaction, i.e., terms such as $\langle C_i' C_j'\rangle$ that arise from cases where R_i is a nonlinear function of

the C_i, were neglected in the development of equation (2.6). The conditions for this approximation to be valid will be discussed in Chapter IV.

Lagrangian Approach

The Lagrangian approach to turbulent diffusion is concerned with the behavior of representative fluid particles. The development of a general equation for the mean concentration $\langle C(x,t)\rangle$ follows that of Seinfeld [22].

$$\langle C(x,t)\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} Q(x,t/x_o,t_o)\langle C(x_o,t_o)\rangle dx_o + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{t_o}^{t} Q(x,t/x',t')S(x',t')dt'dx' \quad (2.7)$$

where $Q(x,t/x^*,t^*)$ is the transition probability density for the particle, that is, the probability density that if the particle is at a position x^* at time t^* will undergo a displacement to x at t, and $S(x,t)$ is the spatial-temporal distribution of particle sources.

Therefore, the first term on the right-hand side of equation (2.7) represents those particles present at t_o, and the second term on the right-hand side accounts for particles added from sources between t' and t.

As can be observed from equation (2.7), the applicability of the Lagrangian approach rests on the ability to

evaluate the transition probability Q. This is a difficult task because complete knowledge of the turbulence properties required to determine Q is generally not available. This problem has been usually overcome by assuming that Q obeys a multidimensional Gaussian distribution, but it is known that this assumption is valid only if the turbulence is stationary and homogeneous. By using that assumption then, one is limited to apply the Lagrangian approach only to some atmospheric cases.

Moreover, the development of equation (2.7) was done for cases where the particles were not undergoing chemical reactions. First-order reactions can be included rather easily in the development of a similar equation, but there is no convenient way of incorporating nonlinear chemical reactions in the Lagrangian approach to turbulent diffusion.

The Eulerian method is very useful in air pollution modeling because the Eulerian statistics are easy to measure and as it will be seen later, possible to represent in an analytical form suitable for computer programs. In addition, the mathematical expressions can be directly applied to situations where chemical reactions take place.

Unfortunately, the Eulerian approach can be solved only by approximate solutions, e.g., the K-theory, and this leads to the problem of accurately predict the eddy diffusivities.

The main objective of the present work is to obtain a model which can be applied to any atmospheric dispersion problem with chemical reactions. Because of the previous analysis of the two approaches that can be used to describe atmospheric diffusion, it was decided to use the Eulerian method as the basis of the present model. As will be seen later, this is the most common approach used although it leads to limited success. The reason being the numerical techniques with which the equations have been solved. Another objective of the present work is to investigate the possibility of a better numerical method for solving the general diffusion equation.

Chapter III

REVIEW OF PREVIOUS WORK

Eulerian Models

The basic mathematical statement for description of the temporal and spatial distribution of chemical species by this approach is the mass balance or continuity equation. This expression, equation (2.6) in this study, plus the appropriate initial and boundary conditions complete the general description.

Exact solutions to this set of equations have not been published. However, it is possible to obtain approximate solutions using numerical techniques.

During the past years, several models have been presented in the literature, ranging from very simple ones like the box model to general cases solved by finite-difference techniques.

Box Model

The simplest air pollution model, though not the first, is the box model, which has been discussed by Sklarew [25]. This model consists of an imaginary box which bounds the atmosphere over a city with the top of the box being at a constant mixing height, the height at which there is no further vertical diffusion. The concentration in the box

is calculated from a simple material balance on the air flow and pollutant emissions, thus, it is not sufficient for anything more than gross estimates, by offering a quick result for long-term concentrations.

Grid Model

Sklarew [25] proposed a different approach on urban air pollution modeling, the grid model. In this model, the region of interest is divided into a three dimensional grid of cells where the diffusion equation of the Eulerian approach is solved. The time-dependent solution is obtained numerically from difference equations.

Lagrangian particles representing a definite amount of pollutant are advected and diffused through the Eulerian grid. In order to do this, a pseudo-velocity $\underset{\sim}{v}^*$ is defined as

$$\underset{\sim}{v}^* = \bar{\underset{\sim}{u}} - D' \underset{\sim}{\nabla} C/C \qquad (3.1)$$

where D' is a diffusivity tensor and $\bar{\underset{\sim}{u}}$ is the wind velocity averaged throughout the cell surrounding each grid point. The defined $\underset{\sim}{v}^*$ then is just the sum of the wind velocity and the velocity corresponding to the diffusion flux. Therefore, the diffusion equation is reduced to

$$\frac{\partial C_i}{\partial t} = - \underset{\sim}{\nabla} (\underset{\sim}{v}^* C_i) + R_i + \text{sources} \qquad (3.2)$$

This equation is solved in time-steps in the following sequence: the pollutant concentration in each cell of the grid is given by the particles in the cell. The cell average concentration is updated by advancing the chemical reactions for a time-step and by adding (and/or substracting) pollutant from sources (and/or sinks) within the cell. Finally, the Lagrangian particles are advected and diffused using the pseudo-velocity, and thus transported at the boundary of each cell for a specific period of time.

As it can be observed, this model is a mixture of the Eulerian and Lagrangian approaches. In spite of being a more general model as compared to the previous one, it has the disadvantage that the grid size necessary for a desired accuracy can result in prohibitive computing time.

Two Dimensional Unsteady State Models

Much of the recent work on air pollution modeling centers on solving a simplified diffusion equation, a two dimensional unsteady state case, which includes only the x-component of the wind velocity and the vertical turbulent diffusion coefficient. In almost all these models, the solutions are obtained by using a finite-difference technique.

For these cases, equation (2.6) for a single species becomes

$$\frac{\partial \langle C \rangle}{\partial t} + \bar{u} \frac{\partial \langle C \rangle}{\partial x} = \frac{\partial}{\partial z} \left\{ K_z \frac{\partial \langle C \rangle}{\partial z} \right\} \tag{3.3}$$

Runca and Sardei [21] solved equation (3.3) using a mixed Lagrangian-Eulerian finite difference scheme. In this model, the emission rate of the source is taken as a boundary condition. The wind velocity and diffusion coefficient are considered to be only functions of z.

Equation (3.3) is solved with the method of fractional steps: the concentration field at time $t+\Delta t$ is obtained from that at time t by separating the contributions due to the advection and diffusion terms of equation (3.3).

In the first step, the following advection equation is solved by a Lagrangian technique over the time interval Δt with the concentration field at time t as initial condition:

$$\frac{\partial C}{\partial t} + u(z) \frac{\partial C}{\partial x} = 0 \tag{3.4}$$

The diffusion equation,

$$\frac{\partial C}{\partial t} - \frac{\partial}{\partial z} \left\{ K_z(z) \frac{\partial C}{\partial z} \right\} = 0 \tag{3.5}$$

the second step, is solved with a conventional Eulerian finite-difference scheme over the same time interval. The initial condition is provided by the concentration field obtained from the first step, and the solution of the second step is an approximation of the concentration field at time $t+\Delta t$.

A different model was presented by Egan and Mahoney [6], where equation (3.3) was also solved, but the source emission rate Q, was included in the same governing equation:

$$\frac{\partial C}{\partial t} + \bar{u}\,\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\{K_z\,\frac{\partial C}{\partial z}\} + Q \qquad (3.6)$$

To simulate transport through an urban area, the region was divided into a number of grid elements, and the partial derivatives in equation (3.6) were approximated by finite differences corresponding to the dimensions of the urban grid elements. Equation (3.6) was solved by an unconventional scheme using moments of concentration distribution.

A slightly more difficult diffusion equation was solved by Eschenroeder and Martinez [7]. A simplified chemical kinetic scheme was included in the governing equation,

$$\frac{\partial C_i}{\partial t} + \bar{u}\,\frac{\partial C_i}{\partial x} = \frac{\partial}{\partial z}\{K_z\,\frac{\partial C_i}{\partial z}\} + R_i \qquad (3.7)$$

$$i = 1, 2, \ldots, s$$

where R_i is the production rate for the ith species and s is the number of species.

The numerical solution of equation (3.7) followed a Crank-Nicholson type implicit finite difference scheme. Since fields for $\bar{u}$ and K_z were prescribed by meteorology inputs, the nonlinearity was confined only to some members of the R_i terms. In a later paper, Eschenroeder and

Martinez [8] reported that a number of difficulties were encountered in using the Crank-Nicholson method and the approach was abandoned.

General Solutions

Some recent work has been done to solve the general expression of the diffusion equation. One of these models was developed by Roth et al [20]. The governing equation solved was the following:

$$\frac{\partial \langle C_i \rangle}{\partial t} + \bar{u}\frac{\partial \langle C_i \rangle}{\partial x} + \bar{v}\frac{\partial \langle C_i \rangle}{\partial y} + \bar{w}\frac{\partial \langle C_i \rangle}{\partial z} = \frac{\partial}{\partial z}\left\{K_z \frac{\partial \langle C_i \rangle}{\partial z}\right\} + R_i(\langle C_1 \rangle, .., \langle C_s \rangle) + Q_i(x,y,z,t) \qquad (3.8)$$

$$i = 1, 2, \ldots, s$$

where K_z is the vertical eddy diffusivity, R_i is the rate of formation of species i by chemical reaction, and Q_i is the rate of emission of species i from sources.

Equation (3.8), plus initial and boundary conditions, was applied for the prediction of pollutant concentrations over a fifty mile square area. This region was divided into a grid of 625, 2x2 mile squares, where 198 grid squares were source-free. The grid actually used in the solution of equation (3.8) was a three-dimensional array of ten layers of cells occupying the space between the ground and the inversion base. Therefore, each cell had a two mile square base and a height of (H-h)/10, being H and h the elevations

of the inversion base and ground above sea level, respectively.

To represent the surface winds, Roth et al. constructed maps of wind speed and wind direction for hourly time intervals, using data gathered at the network of ground-based monitoring stations. In the absence of wind field aloft data, the surface values were used as the basis to calculate wind velocities to all levels between the ground and the inversion base.

A model for the vertical turbulent diffusivity was developed based on the work done by Eschenroeder and Martinez [7].

Finally, the model was completed by a simplified kinetic mechanism involving 12 species and 14 reaction steps. The mathematical representation included four coupled nonlinear differential equations (five other species were expressed by steady-state relations, and the remaining three species were products that could have also been represented by differential equations, but it was not done) that were solved by a modified Gear's method.

A fractional step finite-difference method was selected to be the numerical technique for the model. In this type of solution, a multidimensional problem is replaced by a succession of simpler lower dimensional problems. Therefore, the four-dimensional partial differential equation (3.8) in

(x,y,z,t) was split into three two-dimensional equations in (x,t), (y,t), and (z,t), with the inclusion of the reaction and elevated source terms in the (z,t) fragment. The solution in (z,t) is implicit, while the solution in (x,t) and (y,t) is explicit. Each of these two-dimensional equations was then integrated in succession over one time step, and the terms in each of the three partial differential equations was approximated by finite-difference expressions.

It should be pointed out that this model cannot handle point or line sources, the emissions therefore averaged over relatively large distances.

Another recent model in which a solution to the general expression of the diffusion equation was obtained, was developed by Shir and Shieh [24]. This model was used to study SO_2 distributions in the St. Louis metropolitan area during 25 consecutive days. The region of interest was divided into a three-dimensional grid system of 30x40x14 = 16,800 grid points. The horizontal grid sizes Δx and Δy were of 1524m and the vertical size 20m, 25m, or (H-200)/4 m, values depending on the heights of the vertical grids (H represents the mixing height). The horizontal grid sizes were chosen according to the grid size of the emission source inventory.

The equation solved in this model was the diffusion equation for a single species,

$$\frac{\partial C}{\partial t} + \nabla \, VC = K_H \nabla_H^2 C + \frac{\partial}{\partial z}\{K_v \frac{\partial C}{\partial z}\} + Q + R \qquad (3.9)$$

where C is the mean concentration of SO_2, V = (u,v,w) is the mean wind vector, Q is the source strength rate, R is the chemical reaction rate, K_H is the horizontal eddy diffusivity, and K_V is the vertical eddy diffusivity.

The hourly averaged surface wind field for the total region was obtained by using a weighted interpolation scheme. Data collected at some stations were interpolated to a square grid, which had a size of five area source dimensions. From this wind field, a linear interpolation was used to obtain a wind vector at each grid point.

Since upper layer wind data were not available, the vertical wind profiles at each grid location was assumed to be of power law from

$$V = V_s \, (\frac{z}{z_s})^p \qquad (3.10)$$

where V and V_s are the upper and surface wind at the height z and z_s, respectively. The power constant p was determined by using equation (3.10) and data gathered at heights of 140m and 39m. The vertical component of the wind vector was calculated from the horizontal winds through the continuity equation. Finally, a constant wind direction with height was assumed in the model.

A turbulence transport model developed by Shir [23] was used to calculate the eddy diffusivities. Under neutral conditions, the vertical component of the eddy diffusivity vector is expressed as

$$K_v = u_* \ell \quad , \quad \ell = k_o z \exp(-\frac{4z}{H}) \tag{3.11}$$

where u_*, k_o and H are the friction velocity, the von Kármán constant, and the height of the boundary layer, respectively.

Under non-neutral conditions, an eddy diffusivity, K_s, at the surface layer (z=10m) is calculated using another model, and then extrapolated to higher altitudes by the assumption that

$$K_v = K_s \frac{\ell}{\ell_s} \tag{3.12}$$

In this model, the horizontal eddy diffusivity was assumed to be constant.

Finally, the time-dependent source emission rate was averaged over a 2-hour period for each source, and the chemical reaction rate of SO_2 expressed by

$$R = -kC \tag{3.13}$$

where k is the reaction rate constant with a given value of 10^{-4} sec^{-1}.

A second-order, central finite-difference scheme was used to integrate the advection and horizontal terms, and

the Crank-Nicholson method was used for the vertical diffusion term.

In this model, 2-hour and 24-hour averaged variations of SO_2 concentrations for the 25-day period were obtained, and compared with experimental measurements for the same term average concentrations, at 10 monitoring stations. In their analysis of the results, Shir and Shieh concluded that the 2-hour data were consistently larger than the 24-hour data.

Statistical Models

As it was previously discussed, one of the problems in the Lagrangian approach is the evaluation of the transition probability density function. The most common way that has been used to overcome this problem has been to assume that the transition probability density function, $Q(x,t/x^*,t^*)$ obeys a Gaussian distribution. This assumption has given rise to several models, which will be discussed next.

Gaussian Plume Models

The best known of the practical models based on statistical theory is the Gaussian Plume model. This model was the first recognized continuous point source air pollution model. Most of the existing urban air pollution models are Gaussian Plume models. The concentration of

gas or aerosols at a point (x,y,z) due to a continuous source with an effective emission height L, is given by

$$\langle C(x,y,z)\rangle = \frac{Q}{2\pi\sigma_y\sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \times \left(\exp\left[-\frac{1}{2}\left(\frac{z-L}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+L}{\sigma_z}\right)^2\right]\right) \quad (3.14)$$

The following assumptions are made:

1) The dispersion process is at steady state conditions.
2) The plume spread has a Gaussian distribution in both the horizontal and vertical planes, with standard deviations of plume concentration distribution σ_y and σ_z, respectively, which are function of only the atmospheric stability and distance x from the source.
3) The mean wind speed affecting the plume, u, is oriented in the x-axis and is a constant value for any height.
4) A constant emission rate of pollutants, Q.
5) A total reflection at the earth's surface.
6) No wind shear; and
7) The pollutants are chemically non-interacting.

Typically then, in these models the rate of dispersion is a function of the atmospheric stability class and the travel time or distance from the source. The lateral and vertical distributions are assumed to be Gaussian around the plume centerline. The relation between the horizontal and vertical dispersion coefficients, σ_y and

σ_z, and the Pasquill-Gifford stability categories and downwind distance from the source can be found in Turner [30].

It can be observed then that the Gaussian Plume formula is not flexible enough to include all possible variations that the air motion experiences under urban atmospheric conditions.

Gaussian Puff Models

To describe more accurately the general unsteady state atmospheric diffusion case, some Puff models have been developed by Roberts et al [19] and others. In a Puff model, source emissions are broken into a series of instantaneous puffs instead of a continuous plume. The distribution within a puff is assumed Gaussian in the three directions.

In the Puff model, the entire cloud or puff is assumed to be simultaneously transported along a trajectory given by the mean flow. It is also assumed that the constant standard deviations (or diffusivities) are independent of height, up to an inversion height, that there is no wind shear, and that the pollutants are chemically non-interacting.

Monte Carlo Methods

In a Monte Carlo method, averages of a desired quantity, in this case concentration, are obtained by repeating the process many times using the same initial conditions. Each repetition is called a realization and is controlled by the random forces acting during its particular flight.

A recent model using a Monte Carlo method was developed by Bullin [4]. In this model, the turbulent diffusion process was simulated by allowing a large number of particles representing a definite amount of pollutant to diffuse through the flow field according to the following stochastic Markovian equation

$$\frac{dx_j}{dt} = u_j(x_j,t) + \left[\frac{2D}{P_j}\right]^{1/2} N_j(t) \qquad (3.15)$$

where u_j is the instantaneous velocity in the jth direction, D is the molecular diffusivity, N_j is the jth independent Gaussian white noise with zero mean, P_j is the power spectral density of the jth white noise, and the subscript j denotes the three coordinate directions in the Cartesian space.

After a specified time, the location of each particle was recorded and the concentration distribution was calculated by counting the number of particles within cells of specified size and dividing by the cell volume.

This model was solved on a hybrid computer, where equation (3.15) was programmed for repeated solutions on an analog computer with stochastic variables u_j and N_j being provided as inputs.

As it can be observed, the Gaussian distribution assumption was again incorporated in the model, and no reactions were involved in the simulation of turbulent diffusion in the atmosphere.

Chapter IV

ORTHOGONAL COLLOCATION

In view of all air pollution problems and the need for air quality improvement, air pollution modeling has great practical importance. This is the reason why much consideration has been given to this subject during recent years.

Several air pollution models have been developed so far, but since this subject is very complex, most of those models have been simplified. It is evident that the more simplifications included the less applicable a model is and the poorer the results can be.

It is well known that a major factor that characterizes diffusion processes in the atmosphere is the state of atmospheric turbulence. A general model which includes temporal and spatial variations of meteorological parameters can provide a good description of atmospheric diffusion processes.

As it was discussed in Chapter II, the Eulerian approach will be used for solving the atmospheric diffusion problem in the present work.

A finite-difference scheme has been the most widely used numerical technique for solving the partial differential equations resulting from a model based on the

Eulerian approach. The application of this technique to a general problem gives rise to a very complex model, usually with a large number of grids and in most of the cases then requires much computer time to obtain accurate results. In addition, most of those models cannot handle point sources, and artificial diffusion errors are usually present in the results.

There is a need then to keep working with the diffusion equation in its more general from as a tool for solving air pollution problems, and to investigate the feasibility of using another type of numerical technique which could have better properties than the finite-difference method. This new technique, orthogonal collocation, is discussed next.

Theory

The orthogonal collocation method belongs to the class of weighted residual methods. It was presented by Villadsen and Stewart [31], Finlayson [11], and Villadsen [32], who give details about its theory, some of which will be presented next. They also discuss several applications, mainly one or two-dimensional problems.

The method of weighted residuals is a general method of obtaining solutions to differential equations. The unknown solution is expanded in a set of trial functions, which are specified, but with adjustable constants (or

functions), which are chosen to give the best solution to the differential equation.

The trial function is chosen in such a way that will satisfy the boundary conditions for all selections of the adjustable constants. This trial function then is substituted into the differential equation forming a residual. If the trial function were the exact solution, the residual would be zero. In the weighted residual method, the adjustable constants are chosen so that the residual is forced to be zero in an average sense.

Let us begin considering a boundary-value problem in one independent variable, x. A general type of differential equation can be written as

$$\begin{aligned} L^V(y) &= 0 \qquad \text{in } V \\ L^S(y) &= 0 \qquad \text{in } S \end{aligned} \tag{4.1}$$

where x is the position vector and S the surface or boundary. In the collocation method, the dependent variable y is approximated by a series expansion containing N undetermined parameters. These parameters are then calculated by applying equation (4.1) at N pre-selected points.

In the orthogonal collocation method, the series expansion consists of a set of orthogonal polynomials and the collocation points are chosen as the zeroes of the

polynomials, which make the weighted residuals to be zero in an average sense.

Therefore, for the system given by equation (4.1), the solution is approximated by

$$y(x) = y_o(x) + \sum_{i=1}^{N} a_i P_i(x) \tag{4.2}$$

where $$P_i(x) = \sum_{j=0}^{i} c_j x^j \tag{4.3}$$

is a polynomial such that successive polynomials are orthogonal to all polynomials of order less than i, with respect to some weighting function $w(x) \geq 0$:

$$\int_a^b w(x) P_n(x) P_i(x) dx = 0 \quad , \; n=0,1,\ldots,i-1 \tag{4.4}$$

Depending on the weighting function w(x) and the interval $a \leq x \leq b$, several types of polynomials can be obtained. Choosing $w(x) = 1$, $a = -1$, $b = 1$, and the first polynomial $P_o(x) = 1$, the resulting polynomials, $P_i(x)$, are called Legendre polynomials.

If the weighting function is defined as

$$w(x) = (1-x)^{\alpha}(1+x)^{\beta} \tag{4.5}$$

and the same previous interval is used, the Jacobi polynomials, $P_i^{(\alpha,\beta)}(x)$, are obtained [1]. It follows then that

$$P_i(x) = P_i^{(0,0)}(x) \tag{4.6}$$

The polynomial $P_i(x)$, as defined by equation (4.3), has i roots in the interval $a \leq x \leq b$, which serve as collocation

points. From now on, let N equal the number of those interior collocation points.

Let us now consider polynomials which have additional convenient properties: the solution of a problem is sought in the domain $0 \leq x \leq 1$ and is required to be symmetric about $x=0$. Then, it can be expanded in terms of powers of x^2. A suitable trial function is

$$y(x) = y(1) + (1-x^2) \sum_{i=0}^{N-1} a_i P_i(x^2) \tag{4.7}$$

where the a_i are undetermined constants and the $P_i(x^2)$, polynomials of degree i in x^2 that can be constructed using an orthogonality condition like equation (4.4):

$$\int_0^1 (1-x^2) x^{a-1} P_n(x^2) P_i(x^2) dx = G_i \delta_{in} \tag{4.8}$$

$$n = 1,2,\ldots,i-1$$

where a = 1,2,3, for planar, cylindrical, or spherical geometry.

The polynomials defined by equation (4.8) are Jacobi polynomials [20], and the constant G_i is given by

$$G_i = \frac{[\Gamma(\frac{a}{2})]^2 \Gamma(i+1) \Gamma(i+2)}{(4i+a+2) \Gamma(i+\frac{a}{2}) \Gamma(i+\frac{a}{2}+1)} \tag{4.9}$$

The coefficients of orthogonal polynomials in a new interval $0 \leq x \leq 1$ can also be computed from the old interval polynomials, $-1 \leq x \leq 1$, by the following relation [23]:

$$\text{If} \quad f_i(x) = \sum_{j=0}^{i} c_j x^j \quad , \quad f_i^*(x) = f_i(2x-1) = \sum_{j=0}^{i} c_j^* x^j \tag{4.10}$$

where $f_i^*(x)$ stands for the shifted polynomial. It should be pointed out that if the interval of orthogonality is changed, the weighting function w(x) changes for the Jacobi polynomials, and remains the same (=1) for the Legendre polynomials.

A set of N equations is needed in order to determine the N coefficients a_i, and therefore completely define the solution in the form of the trial function. This can be obtained by substituting equation (4.7) into the differential equation (4.1) and setting the residual formed equal to zero at the N collocation points x_j. These points are the roots to the Nth polynomial, $P_N(x^2) = 0$ at x_j.

The application of the method as described above becomes more confused as N increases (and also if the dimension of the differential equation increases). As a simpler and more attractive alternative to this method, as it will be seen later, the collocation equations can be obtained in terms of the solution at the collocation points, $y(x_j)$. In this method, if the solution at a different point than a collocation point needs to be obtained, it has to be interpolated by using all the known values of $y(x_j)$ at the collocation points.

For this purpose, equation (4.7) can be rewritten as

$$y(x) = \sum_{i=1}^{N+1} d_i \, x^{2i-2} \tag{4.11}$$

where the d_i are undetermined coefficients and the (N+1) collocation point is at x=1. If equation (4.11) is evaluated at the collocation points, the following expression is obtained:

$$y(x_j) = \sum_{i=1}^{N+1} x_j^{2i-2} d_i \tag{4.12}$$

The same procedure can be done for the first derivative and the Laplacian,

$$\frac{dy}{dx}\bigg|_{x_j} = \sum_{i=1}^{N+1} \frac{dx^{2i-2}}{dx}\bigg|_{x_j} d_i \tag{4.13}$$

$$\nabla^2 y\big|_{x_j} = \sum_{i=1}^{N+1} \nabla^2(x^{2i-2})\,\big|_{x_j} d_i \tag{4.14}$$

These equations can be rewritten in matrix notation as follows (the square matrices have (N+1)x(N+1) elements):

$$\underset{\sim}{y} = \bar{\bar{Q}}\underset{\sim}{d} \tag{4.15}$$

$$\underset{\sim}{\nabla y} = \bar{\bar{R}}\underset{\sim}{d} \tag{4.16}$$

$$\underset{\sim}{\nabla^2 y} = \bar{\bar{T}}\underset{\sim}{d} \tag{4.17}$$

where

$$Q_{ji} = x_j^{2i-2}\,, \quad R_{ji} = \frac{dx^{2i-2}}{dx}\bigg|_{x_j},$$

$$T_{ji} = \nabla^2(x^{2i-2})\big|_{x_j} \tag{4.18}$$

The first derivative and Laplacian can be written in terms of the solution $y(x_j)$ by solving $\underset{\sim}{d}$ from equation (4.15) and substituting it into equations (4.16) and (4.17):

$$\nabla \underset{\sim}{y} = \overline{\overline{R}}\ \overline{\overline{Q}}^{-1} \underset{\sim}{y} \equiv \overline{\overline{A}} \underset{\sim}{y} \tag{4.19}$$

$$\nabla^2 \underset{\sim}{y} = \overline{\overline{T}}\ \overline{\overline{Q}}^{-1} \underset{\sim}{y} \equiv \overline{\overline{B}} \underset{\sim}{y} \tag{4.20}$$

Finally then, the derivatives can be expressed as

$$\nabla y = \frac{dy}{dx}\Big|_{x_j} = \sum_{i=1}^{N+1} A_{ji} y_i \qquad \text{for } j=1,\ldots,N+1 \tag{4.21}$$

$$\nabla^2 y = \left[\frac{d^2y}{dx^2} + \frac{a}{x}\frac{dy}{dx}\right]_{x_j} = \sum_{i=1}^{N+1} B_{ji} y_i$$

$$\text{for } j=1,\ldots,N+1 \tag{4.22}$$

where a=0,1, or 2 for plane parallel, cylindrical, or spherical symmetry, respectively, and

$$[A_{ji}] = \begin{bmatrix} \left(\frac{dx^\circ}{dx}\right)_{x_1} & \cdots\cdots & \left(\frac{dx^{2N}}{dx}\right)_{x_1} \\ \vdots & & \vdots \\ \left(\frac{dx^\circ}{dx}\right)_{x_{N+1}} & \cdots\cdots & \left(\frac{dx^{2N}}{dx}\right)_{x_{N+1}} \end{bmatrix} \begin{bmatrix} Q \end{bmatrix}^{-1} \tag{4.23}$$

$$[B_{ji}] = \begin{bmatrix} \nabla^2(x^{\circ})\big|_{x_1} & \cdots & \nabla^2(x^{2N})\big|_{x_1} \\ \vdots & & \vdots \\ \nabla^2(x^{\circ})\big|_{x_{N+1}} & \cdots & \nabla^2(x^{2N})\big|_{x_{N+1}} \end{bmatrix} \begin{bmatrix} \\ Q \\ \\ \end{bmatrix}^{-1} \tag{4.24}$$

$$[Q] = \begin{bmatrix} 1 & x_1^2 & \cdots & x_1^{2N} \\ \vdots & \vdots & & \vdots \\ 1 & x_{N+1}^2 & \cdots & x_{N+1}^{2N} \end{bmatrix} \tag{4.25}$$

Integrals of the solution over the volume V can be calculated with high accuracy via the summation formula

$$\int_o^1 f(x)x^{a-1}dx = \sum_{j=1}^{N+1} W_j f(x_j) \tag{4.26}$$

where the quadrature weights are given by

$$[W_j] = [\int_o^1 x^{o+a-1}dx, \int_o^1 x^{2+a-1}dx, \ldots, \int_o^1 x^{2N+a-1}dx][Q]^{-1} \tag{4.27}$$

Examination of equations (4.23), (4.24), and (4.25) reveals that only the collocation points are needed in order to compute matrices A and B. Once the weighting function w(x), the interval of integration $a \leq x \leq b$, and the number of interior points are specified, these collocation points can be easily calculated.

Let us now consider a more general problem, such as the problem being studied in the present work, in which the symmetry property is removed. In this case then, both even and odd powers of x are included in the orthogonal polynomials in the interval 0 to 1.

In first order differential equations, where only one initial condition needs to be satisfied, a suitable trial function can be of the form

$$y(x) = y(0) + x \sum_{i=0}^{N} a_i P_i(x) \tag{4.28}$$

In this case, y is a polynomial of degree (N+1) in x, and (N+1) equations are needed in order to compute the undetermined constants a_i. These equations can be obtained by substituting equation (4.28) into the first order differential equation at the N interior collocation points, and at the end of the interval x=1.

For second-order differential equations, a general expression for the trial function can be of the form

$$y(x) = b+cx+x(1-x)\sum_{i=1}^{N} a_i P_{i-1}(x) \qquad (4.29)$$

This expression contains (N+2) constants that can be determined by N conditions provided by the residuals evaluated at the N interior collocation points, the N roots to $P_N(x)=0$, and two conditions provided by boundary conditions at x=0 and x=1.

If those two boundary conditions were given as y(0) and y(1), equation (4.29) would remain as

$$y(x) = y(0)[1-x]+y(1)x+x(1-x)\sum_{i=1}^{N} a_i P_{i-1}(x) \qquad (4.30)$$

and therefore only N equations, at the N collocation points, are needed to specify the solution, y(x).

In equation (4.28) as well as in equation (4.30), the polynomials are defined by equation (4.4) with a=0 and b=1. A general expression for the weighting function w(x) can be obtained from equation (4.8) in the following way:

$$\int_o^1 (1-u^2)^{\alpha} u^{a-1} P_i(u^2) P_j(u^2)\,du = G_i\,\delta_{ij} \qquad (4.31)$$

Substitute $x=u^2$, $dx=2udu$:

$$\int_o^1 (1-x)^{\alpha} x^{\frac{a}{2}-1} P_i(x) P_j(x)\,dx = 2G_i\,\delta_{ij} \qquad (4.32)$$

or

$$\int_o^1 (1-x)^{\alpha} x^{\beta} P_i(x) P_j(x)\,dx = G_i^*\,\delta_{ij} \qquad (4.33)$$

Therefore, for a non-symmetric problem, the weighting function is

$$w(x) = (1-x)^{\alpha}x^{\beta} \tag{4.34}$$

This weighting function, as it was discussed before, corresponds to shifted Jacobi polynomials, and it follows then that if $\alpha=\beta=0$, i.e., $w(x)=1$, the polynomials obtained are shifted Legendre polynomials.

In this case, it is also convenient to express the collocation equations in terms of the solution at the collocation points, $y(x_j)$, rather than in terms of the undetermined parameters, a_i. The matrices representing the first and second derivatives, and the approximate expression representing integrals, are given by the same formula as equations (4.19), (4.20), and (4.26), but with different definitions for the elements of the matrices, which now have $(N+2)x(N+2)$ elements:

$$Q_{ji} = x_j^{i-1} \tag{4.35}$$

$$R_{ji} = (i-1)x_j^{i-2} \tag{4.36}$$

$$T_{ji} = (i-1)(i-2)x_j^{i-3} \tag{4.37}$$

In this case, the quadrature weights are

$$[W_j] = [\int_o^1 x^o dx, \int_o^1 x dx, \ldots, \int_o^1 x^{2N+1} dx][Q]^{-1} \tag{4.38}$$

Finally, the derivatives can be expressed in terms of the solution, $y(x_j)$, at the collocation points, following the same procedure as for the symmetrical case, but with different values for matrices A and B:

$$\nabla y = \sum_{i=1}^{N+2} A_{ji} y_i \qquad \text{for } j=1,\ldots,N+2 \qquad (4.39)$$

$$\nabla^2 y = \sum_{i=1}^{N+2} B_{ji} y_i \qquad \text{for } j=1,\ldots,N+2 \qquad (4.40)$$

The procedure to solve a one-dimensional differential equation using this alternative orthogonal collocation method (with matrices A and B) is similar for both, the symmetrical and the non-symmetrical cases. Equations (4.21) and (4.22) for the first case, and equations (4.39) and (4.40) for the non-symmetrical case can be used to express the first and second derivatives in the ordinary differential equation. This equation is then reduced to coupled algebraic equations, with the unknowns being the solutions at the collocation points.

The boundary conditions at x=0 and x=1 can be substituted into those equations so that only N unknowns, at the interior collocation points, and N equations remain to be solved.

As was discussed before, once the interval and the problem are specified (i.e., symmetric or non-symmetric), matrices A and B depend only on the number of collocation

points. If the same number of points is always used in the solution of a problem, these matrices have to be computed only once. Therefore, it might be enough to just include them as input data rather than having a subroutine to calculate them every time the program is run again.

Several tables and some algorithms for the interval $0 \leq x \leq 1$ and different weighting functions and number of collocation points are presented in [1], [11], [31], and [32]. These tables give values of the orthogonal points, matrices A and B, and the quadrature weights W_j for the symmetric case in different geometries, and also for the non-symmetric case.

In order to have more flexibility with respect to the number of points and the weighting function to be used, two subroutines (JCBI and DFOPR presented in Appendix A) were included in the computer program in this study. These algorithms were developed by Michelsen [16].

"JCBI" computes the roots of an Nth degree Jacobi polynomial and the derivatives at these points of the polynomial or the polynomial multiplied by x, by (x-1), or by both (including one or both interval end points x=0 and x=1). In this algorithm, the weighting function is given by equation (4.34).

From the quantities calculated in "JCBI", subroutine DFOPR computes the matrices for the first and second derivatives, and also the quadrature weights.

Let us now consider a more complicated problem, the solution to a two-dimensional differential equation, where the solution ϕ is a function of the independent variables x and y.

The trial function for the symmetrical case (about x=0 and y=0) can be obtained as an extension of equation (4.7). A suitable polynomial expression for $\phi(x,y)$ and subject to the symmetry conditions, and also to the boundary conditions $\phi(x,1) = \phi(1,y) = 0$, is

$$\phi(x,y) = (1-x^2)(1-y^2) \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} a_{ij} P_i(x^2) P_j(y^2) \qquad (4.41)$$

Here, $P_i(x^2)$ and $P_j(y^2)$ are defined in the same way as it was done before, with the use of equation (4.8) for planar geometry.

As has been discussed before, this is not the best way of solving differential equations by orthogonal collocation. It is evident that the confusion becomes worse for two-dimensional problems. Therefore, let us discuss the alternative method where matrices A and B are used. Furthermore, let us analyze non-symmetric cases for being more general cases.

The trial function can be rewritten then as

$$\phi(x,y) = \sum_{i=1}^{N+2} \sum_{j=1}^{M+2} d_{ij} x^{i-1} y^{j-1} \tag{4.42}$$

where N and M are the number of interior collocation points in the x and y directions, respectively.

Let us analyze the x-direction first. Knowing that the partial derivatives with respect to x are at constant y, the following substitution can be made into equation (4.42):

$$e_i = \sum_{j=1}^{M+2} d_{ij} y^{j-1} \tag{4.43}$$

Substituting equation (4.43) into equation (4.42) and evaluating it at the collocation points, x_k, one obtains

$$\phi\Big|_{x_k} = \sum_{i=1}^{N+2} x_k^{i-1} e_i \tag{4.44}$$

The first and second derivatives of equation (4.42) evaluated at the collocation points are

$$\frac{\partial \phi}{\partial x}\Big|_{x_k} = \sum_{i=1}^{N+2} (i-1) x_k^{i-2} e_i \tag{4.45}$$

$$\frac{\partial^2 \phi}{\partial x^2}\Big|_{x_k} = \sum_{i=1}^{N+2} (i-1)(i-2) x^{i-3} e_i \tag{4.46}$$

Using matrix notation, and solving for $\underset{\sim}{e}$ for the first and second derivatives, the previous expressions can be rewritten as

$$\underset{\sim}{\phi} = \bar{\bar{Q}}\underset{\sim}{e} \tag{4.47}$$

$$\frac{\partial \underset{\sim}{\phi}}{\partial x} = \bar{\bar{R}}\bar{\bar{Q}}^{-1}\underset{\sim}{\phi} = \bar{\bar{A}}\underset{\sim}{\phi} \tag{4.48}$$

$$\frac{\partial^2 \underset{\sim}{\phi}}{\partial x^2} = \bar{\bar{T}}\bar{\bar{Q}}^{-1}\underset{\sim}{\phi} = \bar{\bar{B}}\underset{\sim}{\phi} \tag{4.49}$$

where matrices Q, R, and T are defined by equations (4.35) through (4.37).

The same procedure can be used in analyzing the y-direction. One arrives at the same equations (4.47) through (4.49), but changing x_k by y_ℓ, the collocation points in the y-direction, the derivatives now with respect to y, and performing a similar substitution as before,

$$f_j = \sum_{i=1}^{N+2} d_{ij} x^{i-1} \tag{4.50}$$

It follows then that the same A and B matrices can be used for problems in one or two dimensions.

It should be pointed out that in the latter case, after the first and second derivatives and the boundary conditions are substituted into the differential equation, a system of (NxM) algebraic equations remains to be solved.

Partial differential equations can also be reduced to coupled ordinary differential equations, if it is not desired to go further and reduce them to algebraic equations. When both dimensions are collocated, and the differential equation is reduced to algebraic equations, the notation

used (indices) is very important and can give rise to confusion.

Let us illustrate everything that has been said before by setting the collocation equations for an example presented by Villadsen and Stewart [31].

The differential equation and the boundary conditions are:

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = -1 \qquad (4.51)$$

$v=0$ at $x=\pm 1$ and at $y=\pm 1$

This problem is symmetric about x=0 and y=0. Using the matrix B to represent the second derivative, and collocating the same number of points, N, in either direction, the collocation equations are

$$\sum_{i=1}^{N} B_{ji} v_{ik} + \sum_{i=1}^{N} B_{ki} v_{ji} = -1 \qquad (4.52)$$

for $j=1,\ldots,N$

$k=1,\ldots,N$

where the index j represents the x-direction, and k the y-direction. The boundary points $v_{N+1,k}=v_{j,N+1}=0$ have already been substituted into equation (4.52). Equation (4.51) then has been reduced to a system of (NxN) algebraic equations, i.e., equation (4.52).

A similar analysis as done previously can be made for problems in more than two dimensions. It follows that,

as derived before, the same matrices and procedure can be used to reduce partial differential equations to coupled ordinary differential equations or algebraic equations by using the orthogonal collocation method.

Comparison to Finite Difference Techniques

Examination of the orthogonal collocation method, as presented previously, where a problem is solved for the solution at the collocation points rather than for the arbitrary coefficients in the expansion, leads to the conclusion that the equations which must finally be solved are more compact and easier to formulate, than those associated with conventional finite difference techniques.

Once a problem is converted into partial differential equations with the initial and boundary conditions known, and each term in these equations expressed as a funtion of the independent variables, the development of the collocation equations presents no difficulty.

The orthogonal collocation method is therefore a simple numerical technique most suitable for machine computation and with proven fast conversion.

Most of the previous models for solving air pollution problems neglect some of the terms in the general diffusion equation, so that the resulting equation is less complicated to solve. The use of the orthogonal collocation method,

as discussed before, will not introduce extra complications in the formulation of the final equations and their solution if those terms are not assumed to be negligible. Therefore, it will not be more difficult if a general case (four independent variables, the three directions and time) is solved, even with a non-linear reaction term.

Another advantage of the collocation method is that a much smaller number of points may be used since the solution at each point is influenced directly by the value at all the collocation points, as is the case for the exact solution, instead of depending directly on only neighboring grid points as is the case in finite difference schemes. In this respect then, the collocation method requires less computation time than a finite difference solution of comparable accuracy. This has been proved in several applications, some of them discussed next.

Ferguson and Finlayson [9] applied orthogonal collocation to a linear unsteady-state diffusion problem in a slab. They reported that the collocation solution is more accurate than finite difference solutions which use three to twelve times as many spatial grid points (they only collocated in the spatial coordinate and solved the resulting ordinary differential equations).

Ferguson and Finlayson also solved the diffusion of mass and energy in a spherical catalyst pellet with an

exothermic first-order irreversible reaction. Here, they again collocated only in the x-direction and these equations were integrated using Hamming's method. In this case, Ferguson and Finlayson demonstrated that the number of collocation points can be about ten times less than the number of finite difference grid points for equivalent accuracy. In terms of time, the best collocation solution was about twenty times (or more) as fast as a finite difference solution of about the same accuracy.

Finlayson [10] used orthogonal collocation to solve a two-dimensional (axial and radial directions) packed bed reactor under the assumptions of constant physical properties, plug flow, and a reaction governed by the conversion and temperature. Collocation was applied in the radial axis, and the resulting differential equations integrated using the Runge-Kutta method and the Euler method.

Comparison between collocation solutions and finite difference calculations using a Crank-Nicholson implicit method were reported to be in some cases from two to four times faster for equivalent accuracy. In some other cases, the collocation method was twice as fast and ten times as accurate or four times as fast and five times as accurate.

Finlayson [11] also applied collocation in the axial direction in place of the Runge-Kutta method used before, and solved the resulting set of algebraic equations by an iterative procedure proposed by Villadsen [32]. The solution obtained by this way was about three times faster than the one using the Runge-Kutta method for equivalent accuracy.

Finlayson [11] also solved the problem of tubular reactors with only axial dispersion (concentration and temperature). For this case, when orthogonal collocation was applied, the governing equations were reduced to a set of nonlinear algebraic equations for the concentration and temperature at the collocation points. He used the Newton-Raphson method to solve them, and compared this solution to those given in the literature using finite difference schemes.

Finlayson used six collocation points in order to obtain the same accuracy as reported for both a 100-grid point finite difference solution for the isothermal case and 481 grid points for the non-isothermal case.

Application to Turbulent Diffusion in the Atmosphere

As was discussed before, only finite-difference has been used previously to solve for the concentration distribution in atmospheric diffusion processes. The analysis

made in the preceding section leads to the conclusion that air pollution modeling could be improved by the use of the orthogonal collocation method as the numerical technique for solving the general diffusion equation. This equation, for a single species which will be the case studied in the present work[1], is repeated here for convenience.

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}(K_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(K_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(K_z \frac{\partial C}{\partial z}) + R \qquad (4.53)$$

Some of the attractive properties that orthogonal collocation has are its flexibility and easy handling of any variable or component in the diffusion equation, as compared to other numerical methods used in previous works. The model does not increase in difficulty if all the terms involved in equation (4.53) are incorporated in it. That is, a similar amount of work in formulating the collocation equations, but not computer time in solving them, has to be done if three instead of two dimensions are considered in the model. The same reasoning applies for all the components of the wind velocity and turbulent diffusivity, and the chemical reactions. Therefore, it is

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(1) Symbols indicating averaged quantities will be omitted henceforth. All velocities and concentrations, however, continue to be time averaged quantities.

not necessary to assume that some terms are negligible in order to be able to obtain results, which in such a case would be applicable only for some particular situations.

With the present approach then, it is possible to simulate many types of atmospheric conditions. But to do so, it is necessary to express all the properties in equation (4.53) in an analytical form. This has been done in a flexible way by introducing several parameters in the expressions representing those properties, so that different input data can be supplied if different atmospheric conditions are to be tested.

Before applying orthogonal collocation to the present model, let us obtain those expressions for the initial and boundary conditions, turbulent diffusivities, velocity profiles, and chemical reaction.

Initial and Boundary Conditions

The initial conditions necessary for an unsteady state model can be expressed as follows,

$$C = C_B \qquad \text{at } t=0 \quad \text{and any} \quad (x,y,z) \tag{4.54}$$

where C_B is a constant and in general can be a function of x, y, and z.

These conditions are required to start the calculations performed by the integrating subroutine, and therefore are generated in the MAIN of the computer program. For all the cases studied in the present work, there was no background concentration and thus C_B was equated to zero.

The boundary conditions at the ground, z=0, and at the inversion base, z=H, are obtained by assuming that both completely reflect the diffusing pollutant, i.e.,

$$\frac{\partial C}{\partial z} = 0 \qquad \text{at } z=0,H \text{ for any } x \text{ and } y \tag{4.55}$$

These two boundary conditions for the z direction are converted into collocation equations and then incorporated in the diffusion equation, as it will be seen later in this chapter. If for a particular case the gradient in equation (4.55) is not equal to zero, e.g.

$$-K_z \frac{\partial C}{\partial z} = Q_s(x,y,t) \quad \text{at } z=0 \text{ for any } x \text{ and } y \tag{4.56}$$

where $Q_s(x,y,t)$ is the surface flux of the pollutant studied, the collocation equations resulted from conditions (4.55) have to be changed.

The bulk transport of the pollutant is due primarily to the effect of the x-component of the wind velocity. Therefore, it can be assumed that at certain distance in the y-direction, the mean concentration is negligible, i.e.

$$C \rightarrow 0 \quad \text{at } y = -y_{max},\ y_{max} \text{ for any } x \text{ and } z \tag{4.57}$$

where $2 \cdot y_{max}$ is the entire region of interest. In general,

$$C = f(x,z,t) \quad \text{at } y = -y_{max},\ y_{max} \quad \text{for any } x \text{ and } z \tag{4.58}$$

This can also be included in the model by changing the resulting collocation equations from conditions (4.57).

For the purposes of solving equation (4.53), it is necessary to define the location of the sources. These sources can be defined with the aid of a boundary condition in the x-direction.

Let us consider a general case, i.e., a multiple source problem, where there is more than one source involved. If the position of the ith source is defined by the coordinate point (JS(i), KS(i), LS(i)), the boundary condition related to the ith source is given by

$$C = \begin{cases} C_o(i,t) & \text{at } x=JS(i),\ y=KS(i),\ z=LS(i) \\ 0 & \text{at } x=JS(i) \text{ and any other } y \text{ and } z \end{cases} \tag{4.59}$$

where $C_o(i,t)$ is the ith source concentration, and in general a function of time. For the purpose of studying different situations, each C_o, assumed constant in the present model, and its position is supplied as input information. The way of handling multiple source will be discussed in detail in Chapter V.

As a convention, and knowing that for any case there will be at least one source, the first source will always be at x=0, that is JS(1)=0. Therefore, if the problem involves only one source, the boundary condition in the x-direction is given by

$$C = \begin{cases} C_o(1) & \text{at } x=0,\ y=KS(1),\ z=LS(1) \\ 0 & \text{at } x=0 \text{ and any other y and z} \end{cases} \tag{4.60}$$

Sometimes the emission rate (mass/time) and not the source concentration is given as information. This problem can be overcome by the use of quadrature weights in orthogonal collocation and will be discussed later in Chapter V.

There is no need for a second boundary condition in the x-direction, due to the assumption of negligible turbulent diffusivity in this direction. This will be discussed in the next section.

Turbulent Diffusivities, K_j

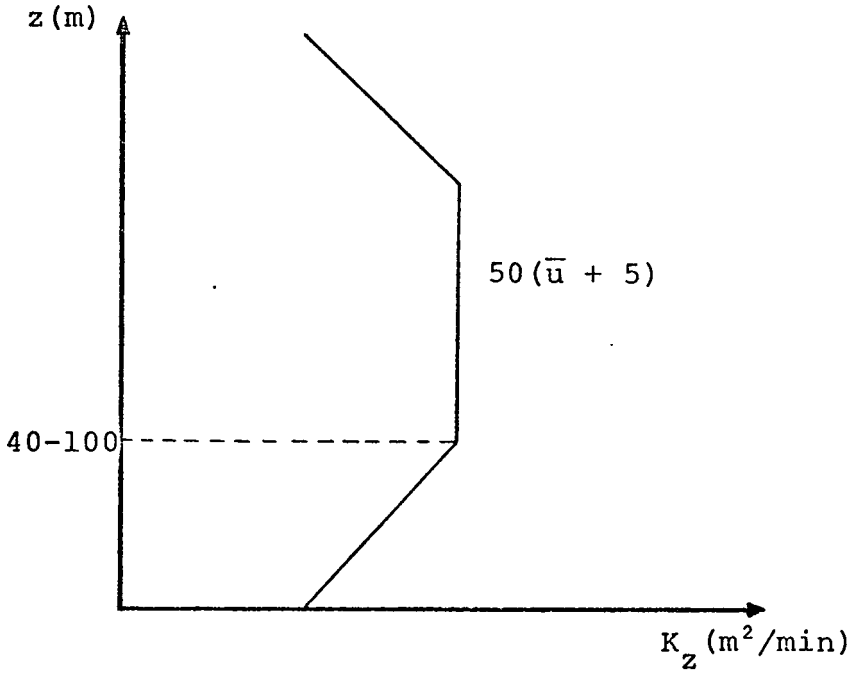
Eschenroeder and Martinez [7] assumed a trapezoidal shaped vertical profile from the ground up to the inversion base for K_z, the turbulent diffusion coefficient in the vertical direction. At low levels, K_z increases linearly with z to some constant value. At intermediate levels, K_z then is constant. As the mixing depth top is

approached, K_z decreases linearly with increasing z. The ground level and inversion layer values are assumed to be equal. The maximum constant value is expected to vary with wind speed approximately like

$$K_z = 50(\bar{u}+5) \qquad m^2/min \tag{4.61}$$

where $\bar{u}$ is in m/s. This equation starts applying from an elevation of 40 to 100 meters, depending upon meteorological conditions:

Figure 4.1: Variations of Diffusivity with Height



Eschenroeder et al. [8] reviewed their previous work based on more experimental data and concluded that equation (4.61) gives an estimate of vertical diffusivity only in the neutral stability range, and that temperature gradients are apparently far more influential than wind speed in determining vertical diffusivity values.

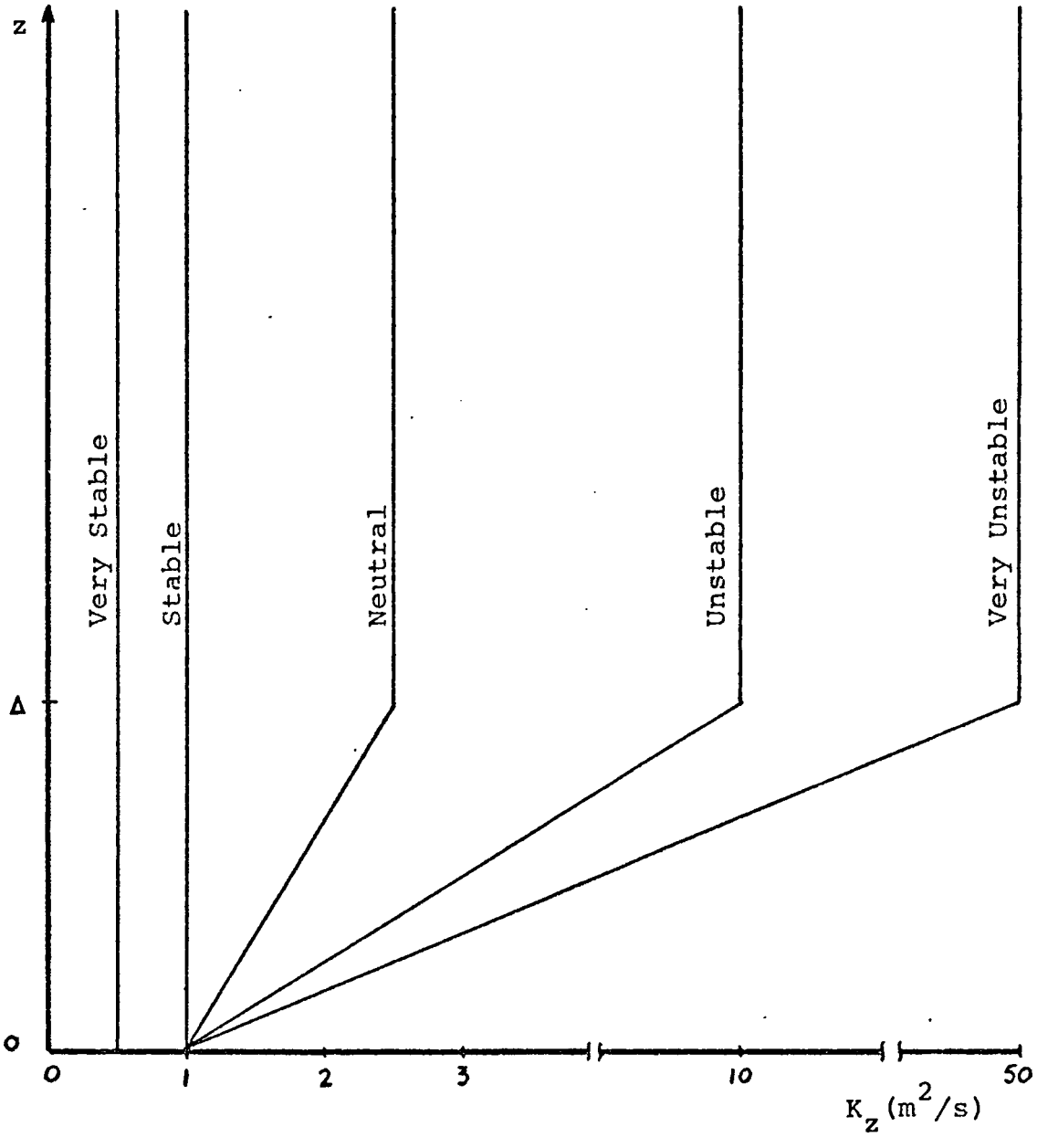
As an improvement on their previous approach, the dependence on wind speed was dropped, and the diffusivity profiles were reconstructed to represent the broad stability categories (defined by Pasquill and Gifford [30]), as shown in Figure 4.2.

The knee height Δ, where the constant values for K_z apply, varies between 25m to 75m above the ground, depending on the height range of the model and the mesh interval size.

Eschenroeder et al. assumed constant diffusivity profiles all the way to the top because of their little influence for the space and time scales in their calculations at the top of the mesh.

In the present model, the calculation procedure for the turbulent diffusivities is based upon the latter approach used by Eschenroeder et al. [8]. Using their approach, K_z will depend only on the stability class and the vertical direction. Some slight changes were made in that approach and are now discussed.

Figure 4.2: Vertical Diffusivity Profiles.
($1 \leq \bar{u} \leq 7$ m/s)



An additional stability class, between the neutral and unstable, was incorporated in the model so that the six classes presented by Turner [13] could be taken into account.

The knee height Δ, was made dependent on the stability class, as suggested by Pasquill [18], so that the more unstable the conditions, the higher the knee.

The last change made to Eschenroeder's approach was to remove their assumption of constant diffusivity profiles from intermediate levels all the way to the top. As the mixing depth top is approached then, the turbulent diffusivities decrease linearly with increasing z, and the ground level and inversion layer values are assumed to be equal. This is done for the last 100 meters of the z-dimension, with $H \geq 300m$.

Taking all these changes into account, Figure 4.2 remains as shown in Figure 4.3.

This model was implemented in the computer program by using the following equations(1):

For ISTB$\leq$4:

K_z = COEFK(ISTB) $\cdot$ z/Δ(ISTB) + 60., for z<Δ(ISTB)

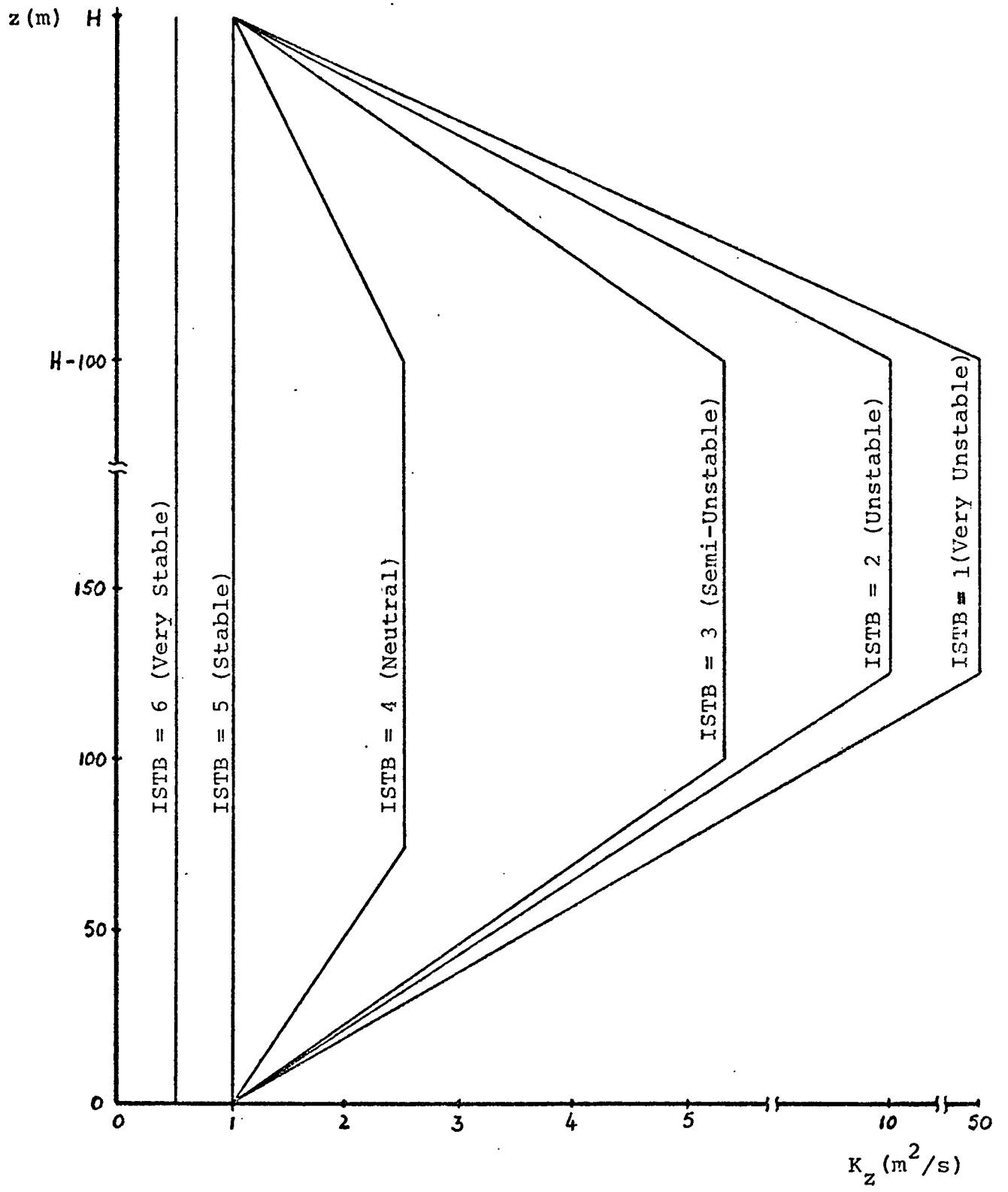
K_z = COEFK(ISTB) + 60., for Δ(ISTB)$\leq$z$\leq$(H-100)

K_z = COEFK(ISTB) $\cdot$ (H-z)/100 + 60., for z>(H-100)

---

(1) In the computer program the units for K_z are m^2/min.

Figure 4.3: Vertical Diffusivity Profiles in the Present Model.



where, COEFK(1) = 2940 $\quad \Delta(1) = 125$

COEFK(2) = 540 $\quad \Delta(2) = 125$

COEFK(3) = 258 $\quad \Delta(3) = 100$ (4.62)

COEFK(4) = 90 $\quad \Delta(4) = 75$

For ISTB = 5: $K_z = 60\ m^2/min$, for any z

for ISTB = 6: $K_z = 30\ m^2/min$, for any z

In order to have a flexible model, the stability class, ISTB, is supplied as input information by the user. Because of the fact that once it is defined it remains the same during the simulation, the algorithm that calculates the turbulent diffusivities at each orthogonal point was incorporated in the MAIN of the computer program.

In the region of interest, the turbulence is almost perfectly isotropic, and even below 100 meters, the degree of isotropy seems to be sufficiently high in order to consider, as Sutton [28] has suggested, that K_y varies in an identical way as K_z. In addition, most of the previous models, discussed in Chapter III, considered a constant turbulent diffusivity in the y direction. This suggested then to relate, in the present model, K_y to K_z in the following manner:

$$K_y = \alpha K_z'(ISTB) \tag{4.63}$$

where α is a positive constant which has to be supplied as input information by the user, and K_z' is the maximum constant value for K_z and thus dependent only on the stability class.

In the present model, the turbulent diffusivity in the x-direction will be neglected as compared to the mean wind velocity. The reason being that its behavior is not well understood and in most of the cases it has no significant effect on the results [24].

Velocity Profiles

Davies [5], Pasquill [17], Smith [26], Tennekes and Lumley [29], and others have developed expressions for the velocity profiles especially in the mean flow direction. Two equation forms have been used often in previous studies. A semi-logarithmic form for rough flows, of the type

$$\bar{u}(z) = \frac{u_*}{k_o} \ln\left(\frac{z}{z_o}\right) \tag{4.64}$$

where u_* is the friction velocity, k_o the von Karman's constant, and z_o a length characterizing the effect of the surface roughness.

The second is a power law equation which has the following form:

$$\bar{u}(z) = \bar{u}_1 \left(\frac{z}{z_1}\right)^m \tag{4.65}$$

where $\bar{u}_1$ is the mean velocity at a reference height z_1, and m is a constant.

For this problem, the latter form describes in a better way the mean velocity in the x-direction. Therefore, equation (4.65) will be used in the diffusion equation.

This form of the velocity profile is used for the lower part of the z dimension, that is from the ground level to the knee height Δ, previously defined, and from this elevation up to the mixing depth top a constant value for the velocity is used, UST. This means then that u will depend on the stability class, z, and the parameters u_1, z_1, m, and UST.

Usually UST, the geostrophic wind speed, is the easiest value to obtain whether by experimental data or previous records of the zone in question. This is the reason why UST is required as input information in the model.

Having in mind further adjustments for u, the constant m has also to be provided as input information by the user. This exponent m is a number which varies from

0.1 to 0.4, depending on the roughness of the ground surface as well as on atmospheric stratification. The rougher the terrain, i.e., the larger the surface obstructions, the thicker will be the affected layer of air, and the more gradual will be the increase of velocity with height. Thus, as the roughness increases, the exponent m increases, as it is shown in Table 4.1 which was presented by Seinfeld [22]:

TABLE 4.1 : ESTIMATES FOR m in eq.(4.65)

	Type of terrain		
	open country	suburbs	urban
m	.16	.28	.40

The stability limits of m, also presented by Seinfeld [22], are:

$$m = \begin{cases} .83 & \text{very stable} \\ 1/7 & \text{neutral} \\ .02 & \text{very unstable} \end{cases}$$

For purposes of continuity calculations (see Chapter V) the ground level value for the mean wind velocity in the x-direction, UGR, is also taken into consideration in the model and is supplied as input information. If its value is not known at the moment of simulating a case,

as it happened in this work, it can be assumed to be equal to the friction velocity, u_*.

The algorithm for obtaining u then, as used in the MAIN program, is described by the following equations:

For ISTB $\leq$ 4:

$$u = UGR \qquad \text{for } z = 0$$

$$u = UST\left(\frac{z}{\Delta(ISTB)}\right)^{AM} \qquad \text{for } 0<z<\Delta(ISTB)$$

$$u = UST \qquad \text{for } z \geq \Delta(ISTB)$$

For ISTB>4 : (4.66)

$$u = UGR \qquad \text{for } z = 0$$

$$u = UST \qquad \text{for } z > 0$$

In almost all the previous works in air pollution modeling, the y-component of the mean wind velocity as well as the z-component are assumed to be negligible.

As it was discussed before, the present model does not increase in difficulty by including more than one component for the mean wind velocity. In spite of this, it has been difficult to obtain equation forms for the other two components of the wind velocity. Therefore, it will be assumed that w, the vertical component is negligible, and that v, the y-component is some fraction of u.

To make a general case for this study, let us consider that v also varies with respect to time in a linear

dependence until it reaches its maximum value. Because of this dependency on time, the algorithm used to its calculation, as described by the following equations, was incorporated in a subroutine called FCT:

$$v = Pu\frac{t}{TCH} \quad \text{for} \quad 0 \leq t < TCH \tag{4.67}$$

$$v = Pu \quad \text{for} \quad t \geq TCH$$

where P is a constant that will determine the direction of the mean wind velocity, and TCH another parameter that will specify the time required for v to change from its value at t=0 to its maximum value, P·u. Both, P and TCH have to be supplied as input information in the computer program by the user.

Chemical Reactions

In the development of equation (2.6), the general diffusion equation, an approximation concerning the chemical reaction term was made: the term $\langle R_i(\langle C_1\rangle + C_1', \ldots\ldots, \langle C_s\rangle + C_s')\rangle$ was replaced by $\langle R_i(\langle C_1\rangle, \ldots, \langle C_s\rangle)\rangle$, i.e., the effect of concentration fluctuations on the rate of reaction was neglected. This is true only for first-order reactions, however, conditions under which this assumption is valid can be obtained for higher order reactions.

Lamb [15] analyzed this problem for a two-dimensional turbulent fluid transporting a single chemical species

involving a nonlinear chemical reaction (second-order reaction). In this case, the chemical reaction term is expressed by

$$R = -k[\langle C\rangle^2 + \langle C'^2\rangle] \tag{4.68}$$

He concluded that the replacement of equation (4.68) by $-k\langle C\rangle^2$ is valid when the reaction process is slow compared with turbulent transport and the characteristic length and time scales for changes in the mean concentration field are large compared with the corresponding scales for turbulent transport.

Although these conditions were derived for a relatively simple two-dimensional case, the essential aspects of those restrictions were found to apply to the general three-dimensional equation as well. In addition, they give a good indication of the conditions of validity for general R_i.

Let us turn our attention now to the mechanisms of removal of sulfur dioxide in the atmosphere, since this will be the chemical species used to validate the present model.

Although a great deal of importance has been given to sulfur oxides, in particular sulfur dioxide, the chemistry of sulfur dioxide in the atmosphere is still far from being fully understood.

The removal of SO_2 in the atmosphere is quite complex and can take place through several mechanisms. It has

been suggested that atmospheric SO_2 can undergo oxidation to sulfates by mainly two mechanisms: catalytic (heterogeneous) oxidation and photochemical (homogeneous) oxidation. However, sulfur dioxide is removed from the atmosphere not only by oxidation, but also by sedimentation, rainout and washout.

Photochemical oxidation of SO_2 is apparently a gas-phase process consisting of several chemical reactions. In the presence of air, SO_2 is oxidized to SO_3 when exposed to solar radiation, and if water is present, the SO_3 is rapidly converted to sulfuric acid. The conversion of SO_2 to SO_3 involves excited SO_2 molecules, oxygen, and oxides of sulfur other than SO_2. Although photochemical oxidation of SO_2 can take place in clean air, the more important process of SO_2 photooxidation occurs in atmospheres containing hydrocarbons and oxides of nitrogen. In this case, the rate of conversion of SO_2 to SO_3 increases markedly over that observed in pure air.

Catalytic oxidation is the principal process for SO_2 conversion under conditions of high humidity and high particulate concentration. It occurs in aqueous solution, involves both water and dissolved O_2, and requires the presence of a catalyst. The overall reaction can be expressed as

$$2SO_2 + 2H_2O + O_2 \xrightarrow{cat.} 2H_2SO_4 \qquad (4.69)$$

Catalysts for this reaction include several metal salts, such as sulfates and chlorides of manganese and iron. However, most of the recent work has been dedicated to manganous salts only.

The same reaction can also occur without the presence of a catalyst, as discussed by Worley [34], and shown in the following equations,

$$SO_2 + H_2O \longrightarrow HSO_3^- + H^+ \text{(seconds)} \qquad (4.70)$$

$$2HSO_3^- + O_2 \xrightarrow{aq.} 2SO_4^= + 2H^+ \text{(hours)}$$

In the sedimentation or deposition process, SO_2 behaves as if it were a particle with a settling velocity. Rainout and washout also serve as additional removing mechanisms. Rainout is the incorporation of gaseous SO_2 in cloud droplets, while washout is the removal of SO_2 by rain falling through air masses below the cloud level. Once SO_2 is absorbed, it is converted via oxidation (4.70)- the heterogenous aspect causes apparent SO_2 level to fall.

As it can be observed, a model that would take into account all the possible mechanisms for SO_2 removal in the atmosphere and all the variables involved would be quite complex.

Because of the fact that the processes previously discussed are not very well understood yet, and the incorporation and thus the study of such a complex model is not the main objective in the present work, only photochemical oxidation will be considered here. Furthermore, the reactions taking place in a system of SO_2, hydrocarbons, NO_x, and air are probably the least well understood of all those in atmospheric chemistry, and thus will not be considered either.

Since data for photochemical oxidation in clean air are extremely scattered, a simplified first order reaction model will be used to represent SO_2 removal from the atmosphere,

$$R = -kC \tag{4.71}$$

where k is the reaction rate constant. The value of 5.8×10^{-5} per minute or 0.35% loss of SO_2 per hour, used by Hallidy and Anderson [12] in their work will be the rate constant in the present model, and must be supplied as input information in the computer program.

Development of the Collocation Equations

The diffusion equation to be solved, and the corresponding initial and boundary conditions, under the assumptions previously discussed, are:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = \frac{\partial}{\partial y}(K_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(K_z \frac{\partial C}{\partial z}) + R \qquad (4.72)$$

$$C = 0 \qquad \text{at } t=0, \text{ and any } (x,y,z) \qquad (4.73)$$

$$\frac{\partial C}{\partial z} = 0 \qquad \text{at } z=0,H \text{ for any } x \text{ and } y \qquad (4.74)$$

$$C^{(*)} = \begin{cases} C_o(1) & \text{at } x=0,\ y=KS(1),\ z=LS(1) \\ 0 & \text{at } x=0, \text{ and any other } y \text{ and } z \end{cases} \qquad (4.75)$$

$$C = 0 \qquad \text{at } y= -y_{max},\ y_{max} \text{ for any } x \text{ and } z \qquad (4.76)$$

In equation (4.72), the velocity profiles are assumed to be,

$$u = \psi(z,ISTB) \qquad (4.77)$$

$$v = \eta(z,t,ISTB) \qquad (4.78)$$

the turbulent diffusivities,

$$K_y = \xi(ISTB) \qquad (4.79)$$

$$K_z = \zeta(z,ISTB) \qquad (4.80)$$

and the rate of reaction,

$$R = -kC \qquad (4.81)$$

For this problem, let us transform the spatial coordinates to yield limits of 0 to 1 by the following procedure:

(*) The multiple sources case will be discussed in Chapter V.

$$x^* = \frac{x}{x_{max}} \tag{4.82}$$

$$y^* = \frac{\frac{y}{y_{max}} + 1}{2} \tag{4.83}$$

$$z^* = \frac{z}{H} \tag{4.84}$$

For simplicity, from now on the asterisk will be dropped out from the independent variables, x*, y*, and z*.

Substituting equations (4.77) through (4.84) into equation (4.72) one obtains

$$\frac{\partial C}{\partial t} + R_1 \frac{\partial C}{\partial x} + R_2 \frac{\partial C}{\partial y} - R_3 \frac{\partial C}{\partial z} = R_5 \frac{\partial^2 C}{\partial y^2} + R_6 \frac{\partial^2 C}{\partial z^2} - kC \tag{4.85}$$

where

$$R_1(z) = \psi(z,ISTB) \frac{1}{x_{max}} \tag{4.86}$$

$$R_2(z,t) = \eta(z,t,ISTB) \frac{1}{2y_{max}} \tag{4.87}$$

$$R_3(z) = \frac{d\{\zeta(z,ISTB)\}}{dz} \frac{1}{H^2} \tag{4.88}$$

$$R_5 = \xi(ISTB) . \frac{1}{4y_{max}^2} \tag{4.89}$$

$$R_6(z) = \zeta(z,ISTB) \frac{1}{H^2} \tag{4.90}$$

There are many ways in which orthogonal collocation can be applied to equation (4.85), but it is chosen to collocate only in the three directions, x, y, and z, so that a system of ordinary differential equations with respect to time is left to be solved. The reason of doing this is because the solution of the diffusion equation is primarily wanted at any instant of time.

If the emission source is put in the middle of the interval in the y-direction, and only the x-component of the wind velocity is taken into account, then by examining the boundary conditions it can be concluded that this problem would be symmetric with respect to y. Since this is only a particular case, it is better to apply the equations for a non-symmetric case to every direction.

In doing this, let N_x, N_y, and N_z be the number of collocation points in the x, y, and z directions, respectively, and $C_{jk\ell}$ the mean concentration at the point (x_j, y_k, z_ℓ).

Equation (4.85) remains then as,

$$\frac{dC_{jk\ell}}{dt} + R_1(\ell) \sum_{i=1}^{N_x+2} A_{ji}^{(1)} C_{ik\ell} + R_2(\ell,t) \sum_{i=1}^{N_y+2} A_{ki}^{(2)} C_{ji\ell} -$$

$$- R_3(\ell) \sum_{i=1}^{N_z+2} A_{\ell i}^{(3)} C_{jki} = R_5 \sum_{i=1}^{N_y+2} B_{ki}^{(2)} C_{ji\ell} +$$

$$+ R_6(\ell) \sum_{i=1}^{N_z+2} B_{\ell i}^{(3)} C_{jki} - kC_{jk\ell} \qquad (4.91)$$

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

As discussed before, matrices A and B depend on the number of collocation points. For a general case, that number of points can be different for each direction and therefore, A and B would be different. Furthermore, N_x, N_y, and N_z could be changed between runs. These reasons lead to the conclusion that it is better to include subroutines JCBI and DFOPR in the computer program rather than putting matrices A and B as input data each time the collocation points are changed.

In equation (4.91), the indices of matrices A and B represent the direction and thus the way they are computed, i.e., (1), (2), and (3) stand for the x, y, and z directions, respectively.

The application of orthogonal collocation to the boundary conditions, equations (4.74) through (4.76), gives the following expressions:

$$\sum_{i=1}^{N_z+2} A^{(3)}_{1i} C_{jki} = 0 \qquad \text{at } z=0 \tag{4.92}$$

$$\sum_{i=1}^{N_z+2} A^{(3)}_{N_z+2,i} C_{jki} = 0 \qquad \text{at } z=1 \tag{4.93}$$

$$C_{1k\ell} = \begin{cases} C_o(1) & \text{at point source} \\ 0 & \text{elsewhere} \end{cases} \tag{4.94}$$

$$C_{j1\ell} = 0 \qquad \text{at } y=0 \tag{4.95}$$

$$C_{jN_y+2\ell} = 0 \qquad \text{at } y=1 \tag{4.96}$$

Equations (4.92) and (4.93) can also be written as

$$A^{(3)}_{11} C_{jk\ell} + \sum_{i=2}^{N_z+1} A^{(3)}_{1i} C_{jki} + A^{(3)}_{1N_z+2} C_{jkN_z+2} = 0 \tag{4.97}$$

$$A^{(3)}_{N_z+2\,1} C_{jk1} + \sum_{i=2}^{N_z+1} A^{(3)}_{N_z+2i} C_{jki} + A^{(3)}_{N_z+2N_z+2} C_{jkN_z+2} = 0 \tag{4.98}$$

Solving for C_{jk1} and C_{jkN_z+2} one obtains:

$$C_{jkN_z+2} = \frac{\sum_{i=2}^{N_z+1} (A^{(3)}_{11} A^{(3)}_{N_z+2i} - A^{(3)}_{N_z+21} A^{(3)}_{1i}) C_{jki}}{A^{(3)}_{N_z+21} A^{(3)}_{1N_z+2} - A^{(3)}_{11} A^{(3)}_{N_z+2N_z+2}} \tag{4.99}$$

$$C_{jk1} = -\frac{A^{(3)}_{1N_z+2} C_{jkN_z+2} + \sum_{i=2}^{N_z+1} A^{(3)}_{1i} C_{jki}}{A^{(3)}_{11}} \tag{4.100}$$

These expressions can be simplified by defining,

$$DEN = A^{(3)}_{N_z+21} A^{(3)}_{1N_z+2} - A^{(3)}_{11} A^{(3)}_{N_z+2N_z+2} \tag{4.101}$$

$$APA1(i) = \frac{A_{11}^{(3)} A_{N_z+2i}^{(3)} - A_{N_z+21}^{(3)} A_{1i}^{(3)}}{DEN} \qquad (4.102)$$

so that equation (4.99) remains as

$$C_{jkN_z+2} = \sum_{i=2}^{N_z+1} APA1(i) C_{jki} \qquad (4.103)$$

In cases where there is no inversion layer at the maximum elevation, H, as it has been assumed so far, a new boundary condition at this point can be assumed as

$$C = 0 \quad \text{at} \quad z=H \quad \text{for any } x \text{ and } y \qquad (4.104)$$

This condition can be easily included in equation (4.103):

$$C_{jkN_z+2} = \sum_{i=2}^{N_z+1} APA1(i)\ C_{jki} \quad INVRS \qquad (4.105)$$

where INVRS=1 means that there is inversion at z=H, and INVRS=0 means that there is no inversion and the concentration at z=H is equal to zero.

By substituting equations (4.94) through (4.96), equation (4.91) remains as follows:

$$\frac{dC_{jk\ell}}{dt} + S(j) + R_1(\ell) \sum_{i=2}^{N_x+2} A_{ji}^{(1)} C_{ik\ell} + R_2(\ell,t) \sum_{i=2}^{N_y+1} A_{ki}^{(2)} C_{ji\ell} -$$

$$- R_3(\ell) A_{\ell 1}^{(3)} C_{jk1} - R_3(\ell) \sum_{i=2}^{N_z+1} A_{\ell i}^{(3)} C_{jki} -$$

$$- R_3(\ell) A_{\ell N_z+2}^{(3)} C_{jkN_z+2} = R_5 \sum_{i=2}^{N_y+1} B_{ki}^{(2)} C_{ji\ell} +$$

$$+ R_6(\ell) B_{\ell 1}^{(3)} C_{jk1} + R_6(\ell) \sum_{i=2}^{N_z+1} B_{\ell i}^{(3)} C_{jki} +$$

$$+ R_6(\ell) B_{\ell N_z+2}^{(3)} C_{jkN_z+2} - kC_{jk\ell} \qquad (4.106)$$

And rearranging,

$$\frac{dC_{jk\ell}}{dt} = -S(j) - R_1(\ell) \sum_{i=2}^{N_x+2} A_{ji}^{(1)} C_{ik\ell} +$$

$$+ [R_3(\ell) A_{\ell 1}^{(3)} + R_6(\ell) B_{\ell 1}^{(3)}] C_{jk1} +$$

$$+ [R_3(\ell) A_{\ell N_z+2}^{(3)} + R_6(\ell) B_{\ell N_z+2}^{(3)}] C_{jkN_z+2} +$$

$$+ \sum_{i=2}^{N_z+1} [R_3(\ell) A_{\ell i}^{(3)} + R_6(\ell) B_{\ell i}^{(3)}] C_{jki} +$$

$$+ \sum_{i=2}^{N_y+1} [R_5 B_{ki}^{(2)} - R_2(\ell,t) A_{ki}^{(2)}] C_{ji\ell} - kC_{jk\ell} \qquad (4.107)$$

or,

$$\frac{dC_{jk\ell}}{dt} = -S(j) - R_1(\ell) \sum_{i=2}^{N_x+2} A_{ji}^{(1)} C_{ik\ell} + R361(\ell) C_{jk1} +$$

$$+ R362(\ell) C_{jkN_z+2} + \sum_{i=2}^{N_z+1} R36I(\ell,i) C_{jki} +$$

$$+ \sum_{i=2}^{N_y+1} R52I(\ell,k,i,t) C_{ji\ell} - kC_{jk\ell} \qquad (4.108)$$

$$\text{for} \quad j=2, \ldots, N_x+2$$

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

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

where

$$S(j) = \begin{cases} R_1(LS(1)) A_{j1}^{(1)} C_o(1) & \text{at } k=KS(1) \\ & \ell=LS(1) \\ 0 & \text{elsewhere} \end{cases} \qquad (4.109)$$

and C_{jk1} and C_{jkN_z+2} are given by equations (4.100) and (4.105), respectively.

Equation (4.108) gives then a set of $(N_x+1)(N_y)(Nz)$ first-order ordinary differential equations to solve for the concentration as a function of time at the orthogonal collocation points in the three directions, x, y, and z.

Chapter V

FORMULATION OF CALCULATIONAL SCHEME

Calculation Procedure

It has previously been shown that the solution to the turbulent diffusion process in the atmosphere can be obtained by the use of the K-theory, which can be accomplished by solving a partial differential equation. Orthogonal collocation simplifies this, reducing that equation to a system of first-order ordinary differential equations with respect to time.

The basic calculational procedure then is to solve that system of equations (4.108) on a digital computer. There are several methods that can be used for this purpose, but in this work it was decided to use RKGS, a subroutine furnished by IBM [14] which in essence is a fourth-order Runge-Kutta method.

In addition to RKGS, two other subroutines must be supplied: A function subroutine, called FCT in the computer program (see Appendix A), where the system of first-order ordinary differential equations to be solved are provided; and an output subroutine, called OUTP in the computer program, which will print the results computed by RKGS.

In RKGS, the integration is performed with respect to time, and therefore the solution of the problem can be obtained at any moment. However, it is usually desired to print it only at every defined interval of time. Having this in mind, an algorithm that uses a variable called PRDEL was incorporated in OUTP so that it will allow the computer to print the results only every PRDEL units of time.

Due to the nature of orthogonal collocation, small oscillations can be introduced in the solution of the problem. Although these are part of the true solution of the collocation equations, there might be small negative concentrations as output for points that follow zero levels of concentration. Because of this, and by suggestions of Stewart [27] and Villadsen [33], a subroutine called ZERO is always called before printing the results. This subroutine will convert all the concentration values that follow the zero level to zero. This testing is done in all three directions.

Because of the fact that actual data are available as average concentrations, the computer program contains a subroutine called AVG, which will convert the solution to a time average solution, so that a comparison to experimental data can be performed. To do this, AVG subroutine computes the time average concentrations at

every collocation point for three consecutive points in time; i.e., Θ, t, and Ω, where t is any point in time, Θ(=t-PRDEL) is the time between the pollutant release(t=0) and the initiation of the averaging time, and Ω(=t+PRDEL) is the end of the averaging time. In order to reduce the program storage requirement, AVG subroutine is performed by direct-access input/output statements.

Multiple sources

In Chapter IV, orthogonal collocation was applied to problems involving only one point source. The same resulting collocation equations can be used to multiple source cases, but the calculational procedure is different.

As it was previously discussed, the concentration at the source is considered here as the boundary condition in the x-direction. If the problem involves only one source, the input information required to solve it consists of C_o(1), the concentration at the source, KS(1) and LS(1), the location of the point source in the y and z directions, respectively (JS(1) in this case is equal to zero, i.e., x=0), and XMAX, YMAX, and H, the dimensions in the three directions. The calculation of the solution starts at TINIT, the initial time and ends at ENDS, the end of the simulation time. Intermediate results are computed at every interval of integration time, PRMT(3),

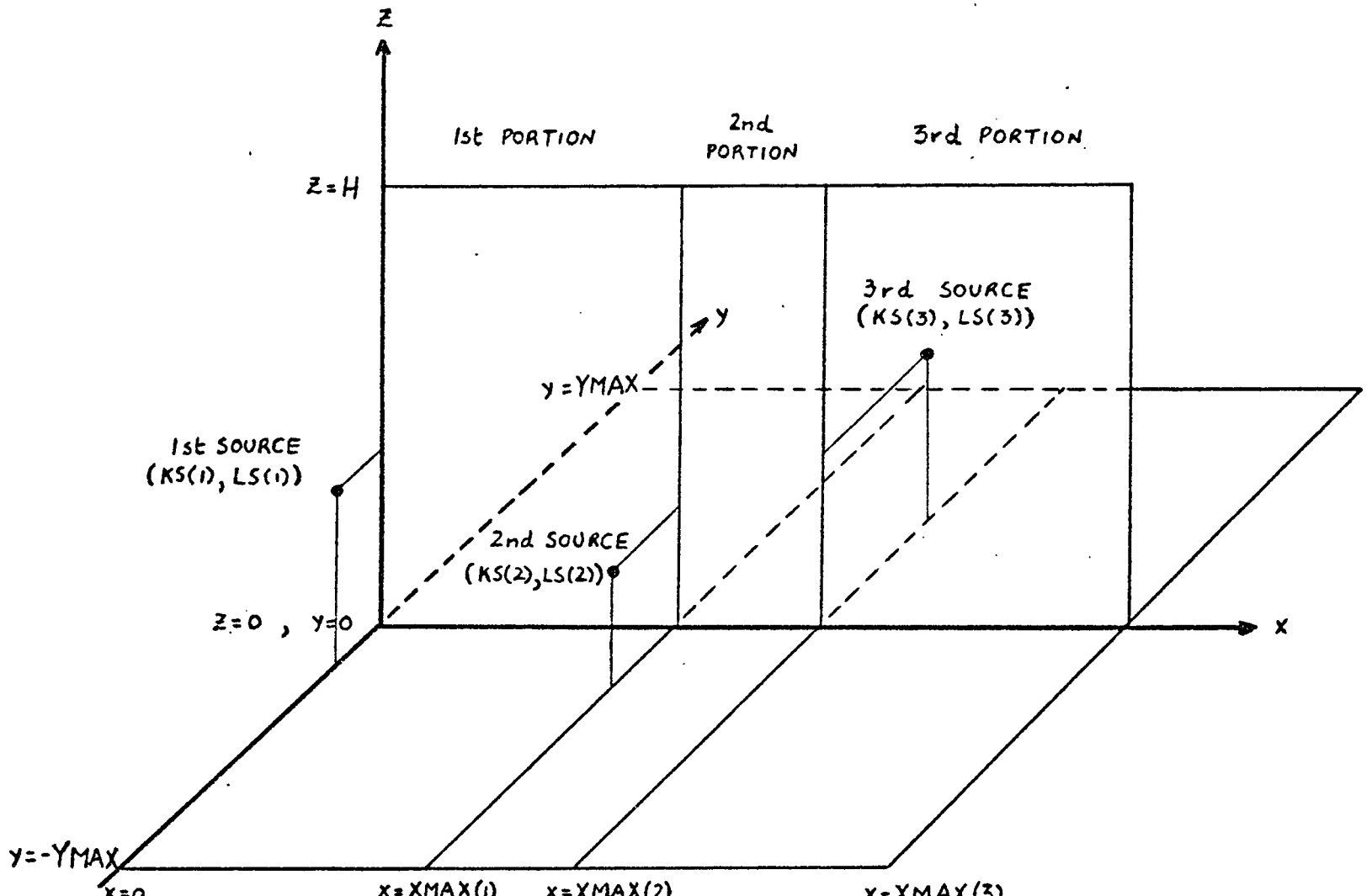
but are printed only every PRDEL units of time. TINIT, ENDS, PRMT(3), and PRDEL are also required as input information.

The calculation procedure for cases involving more than one source is different than the one previously presented. The reason being the interaction that occurs on the concentration distribution due to the multiple sources.

In order to describe the calculation procedure for multiple sources, let us analyze a situation that involves three point sources. In this case, the source concentrations, $C_o(i)$ are still considered as boundary conditions in the x-direction, but while the first source is located at x=0, the following ones can be located in general at x>0. The entire domain in the x-direction is divided into three portions, so that the first source is located at x=0, the second at XMAX(1), and the third at XMAX(2). In order to define completely each source, its position in the y and z directions must be supplied by the values of KS(i) and LS(i), respectively, where i indicates the number of the source. This case then can be represented as it is shown in Figure 5.1.

The input information given by TINIT, ENDS, PRMT(3), PRDEL, NX, NY, NZ, YMAX, and H is the same for each source. The number of sources, NSRCS, must also be supplied as input information, and in the present model

Figure 5.1: Multiple Sources Representation



NSRCS $\leq$ 3. If more than three sources are to be considered, changes should be made in the dimension and common statements, initial conditions, and RKGS call statements.

The results for the first portion of Figure 5.1 are the same as if they were computed for a single source problem, but for the next portions this is different. The concentrations in the second portion not only depend on $C_o(2)$, but also on the mass flux that comes from the first portion. The same reasoning applies for subsequent portions.

The calculation procedure then is as follows: at every interval of integration time, the concentration values at any orthogonal point in the y-z plane at x=XMAX(1) are recorded and used, with $C_o(2)$, as boundary conditions for the second portion. The same procedure is also utilized for the following portions. This method can be implemented in the computer program by two ways: (1) Integrating the three portions at the same time for every interval of time, printing every PRDEL units of time, and continuing to do this until ENDS is reached. This can be done by integrating first the last portion for one interval of time. The values recorded for the preceding portion at the previous interval of time are used as boundary conditions for the interval of time and the portion in question. After this calculation is over,

the same procedure can be applied for the next portion going backwards, and continuing to do this until the first portion is reached. In this way, the same storage can be used to record the values at x=XMAX(1) and XMAX(2) for every interval of time. Furthermore, once the values are printed, the concentration distribution at time=Θ are not used any more and that storage can be utilized for the next PRDEL units of time.

(2) Integrating the first portion between TINIT and ENDS and recording all the values, then integrating the next portion i all the way, using the values at x=XMAX(i-1) for every interval of integration time recorded previously, and continuing to do this until the last portion is reached. Then, at every PRDEL units of time the solution for that portion and the ones in the disk can be printed. The simulation stops when ENDS is reached for that last portion. It is evident that this method will require more storage capacity than the previous one.

An analysis made on both methods indicated less computational time for the latter way. Therefore, the second method was put in the system.

It should be pointed out that the position of any source can be located only at orthogonal collocation points. That position, given by KS and LS, must be supplied with point numbers. For example, if N_Z=7 and

the location of a source is at one half of the z-diamension, LS should be 5 (the total number of collocation points is 9, including z=0 and z=1).

Continuity

In the present model, the concentration at the source, $C_o(i)$, is used to represent the source, and therefore is a required input information. Unfortunately, the emission rate is, in many cases, the only information that is available. One of the objectives of the present study is to obtain a general model that would also compute the concentration distribution when only the emission rate of the source is given.

There is a need then to develop a calculational procedure which would compute a concentration equivalent to the emission rate. The concept of continuity can be used for this purpose. Moreover, the flux at any x is a valuable piece of information that can be obtained from the results of an air pollution model. Therefore, a general continuity calculation will be obtained and then used for the particular problem of computing $C_o(i)$ from the emission rate Q(i).

The flux across any plane normal to the x axis can be expressed by the following equation:

$$\int_{0}^{H}\int_{-YMAX}^{YMAX} C \cdot u \, dydz = Q_{x_j} \tag{5.1}$$

where C is the mean concentration at any point in the y-z plane, u its corresponding x-component of the mean wind velocity, and Q_{x_j} the mass rate at $x=x_j$.

If there was no mechanism of removal in a model involving one source, the pollutant would be not created or lost within the region of interest, and at steady state Q_{x_j} would be the same for any value of x, and equal to Q(1). For a multiple source case, Q_{x_j} would be equal to the sum of the constant emission rates for a particular source and its precedings. In such a case, the continuity condition should be included in the model, but since removal is taken into account in the present study, the values of Q_{x_j} will vary along the x direction.

Transforming the spatial coordinates into an interval between 0 and 1, equation (5.1) remains as follows:

$$\int_{0}^{1}\int_{0}^{1} C \cdot u \, (2 \cdot YMAX \cdot H) dydz = Q_{x_j} \tag{5.2}$$

Using the quadrature weights, the double integral can be transformed into a double summation leading to the following collocation equation

$$\sum_{k=1}^{N_y+2} \sum_{\ell=1}^{N_z+2} W^{(2)}(k) W^{(3)}(\ell) C_{jk\ell} u(\ell) (2 \cdot YMAX \cdot H) = Q_{x_j} \quad (5.3)$$

$$\text{for } j=2, \ldots, N_x+2$$

But from the boundary conditions in the y direction,

$$C_{j1\ell} = C_{jN_y+2\ell} = 0 \qquad j=2, \ldots, N_x+2 \quad (5.4)$$

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

Finally then, equation (5.3) remains as

$$Q_{x_j} = \sum_{k=2}^{N_y+1} \sum_{\ell=1}^{N_z+2} W^{(2)}(k) W^{(3)}(\ell) C_{jk\ell} u(\ell) (2 \cdot YMAX \cdot H) \quad (5.5)$$

$$\text{for } j=2, \ldots, N_x+2$$

Equation (5.5) was included in the model (in subroutine OUTP) so that the mass flux can be known at any time and at any position in the x direction. In a case of no removal, these values, if they were equal as it will be shown in the next chapter, serve as a proof of the validity of the model and the numerical technique used.

In the case of using equation (5.5) to calculate the equivalent $C_o(i)$, Q_{x_j} is equated to the constant rate of emission, $Q(i)$, and all the concentrations but the one at the point source are made equal to zero. Equation (5.5) becomes then

$$Q(i) = W^{(2)}(KS(i))W^{(3)}(LS(i))C_o(i)u(LS(i))(2\cdot YMAX\cdot H) \quad (5.6)$$

for i=1, ..., NSRCS

Therefore, whenever Q(i) is the only information available, the equivalent concentration at the source can be calculated from the following equation:

$$C_o(i) = \frac{Q_{(i)}}{W^{(2)}(KS(i))\ W^{(3)}(LS(i))\ u(LS(i))\ 2\cdot YMAX\cdot H} \quad (5.7)$$

Chapter VI

PRESENTATION AND ANALYSIS OF RESULTS

The objective of the current study was to demonstrate the suitability of the present method to simulate diffusion in the atmosphere. To do this, experimental cases are simulated with the present model, and the results compared to the corresponding experimental data. Unfortunately, at the present moment there are almost no experimental data available in the literature. This is the reason why only the Project Prairie Grass diffusion data at O'Neill, Nebraska, were considered. Four cases from this Project were simulated and the results compared to the experimental data.

In addition, a parametric study was performed, and the sensitivity of the present model to variations in the atmospheric conditions analyzed. This was done by simulating several hypothetical cases.

Comparison to Experimental Values

The atmospheric diffusion data from Runs #20, #24, #45, and #54 of the Project Prairie Grass data [2, 3, 13] were used as a test of the present method.

Project Prairie Grass was a field program designed to provide experimental data on the diffusion of a tracer gas in the atmosphere. The sulfur dioxide tracer gas was released for ten minutes over a flat prairie at O'Neill, Nebraska. The emission was done at about 50 centimeters above the ground and the gas was sampled along semicircular arcs from 50 meters to 800 meters from the source. Samplers were placed at 1.5m above the ground. In addition, concentration profiles along the vertical were measured from samplers located at nine levels on each of six towers positioned along the 100m arc.

In the experiments, the entire sampling network was put in operation just before the start of the gas release and the operation continued until the tracer was transported beyond the 800m arc. Although the actual measurements were of total exposure for each gas release, the investigators reported average concentrations for a ten minute sampling time. It was estimated that the concentration measurements were accurate to within about 10%.

Several meteorological measurements were taken during the tracer release. Among others, the mean wind velocity at two meters above ground. These values were used in the present model to simulate the mean wind velocity profile.

The source strengths Q, and the mean wind velocities at 2 meters u_1, for the four cases simulated in the present study were as follows:

Table 6.1 : Source Strengths and Mean Velocities (at 2m) for Experimental Cases Simulated

Run No.	Q(g/s)	u_1(m/s)
20	101.2	9.38
24	41.2	5.86
45	100.8	6.02
54	43.4	3.94

In the present model, concentration profiles were simulated using the power law equation for the mean wind velocity as

$$\bar{u} = u_1 \left(\frac{z}{z_1}\right)^{.14} \qquad (6.1)$$

where u_1 corresponds to the value given in Table 6.1 for an elevation of z_1 = 2m, and z = elevation in meters.

It can be observed that the source emission rate is the only available information related to the source. Therefore, the equivalent concentration at the source, $C_o(1)$, was calculated using equation (5.7) with the source strength Q(1) given by Table 6.1.

Since no data for the turbulent diffusivities were available, the four cases were simulated assuming $\alpha=1$, i.e., the turbulent diffusivities in the y and z directions were the same; and a stability class 4, i.e., neutral stability. In addition, INVRS was made equal to zero, i.e., no inversion at the maximum elevation; and a first-order reaction with $k = 5.8 \times 10^{-5}$ min^{-1} was assumed for all cases.

In addition to the experimental values, the concentration profiles calculated by the present method were also compared to the ones (#45 and #54) obtained by the statistical method developed by Bullin [4].

Simulated vertical profiles at the centerline for Runs #20, #24, and #45, and at 20m from the centerline for Run #54 (no experimental data for the centerline were available) are compared with the limited experimental data available in Figures 6.1 through 6.4. There is good agreement between experimental and simulated vertical profiles except for Run #45, where the concentration values near ground level were much lower than the experimental ones. The reason for this discrepancy is a higher simulated velocity profile, u_s, as compared to the actual one u_a. This difference, especially near ground level, can be observed in Table 6.2.

Table 6.2 : Comparison Between Actual and Theoretical Values for the Mean Velocity in Run #45

z(m)	u_a(m/s)	u_s(m/s)
0.25	3.78	4.50
0.5	4,60	4.96
1.0	5,31	5.46
2.0	6,02	6.02
4.0	6,65	6.63
8.0	7.35	7.31
16.0	7.88	8.05

Another reason for the discrepance in Run #45 can be due to a possible smaller simulated turbulent diffusivity in the z direction. This was checked by simulating the same problem, but with stability class 3, i.e., semi-unstable. The results are also plotted in Figure 6.3, and it can be observed that the concentration values increased and thus the difference between the experimental and theoretical values decreased.

Horizontal concentration profiles for the four cases at 1.5m above ground and at downwind distances of 200m and 400m are shown in Figures 6.5 through 6.8. In general, the agreement between experimental and simulated values is good.

The mass flux (g/s) across y-z planes at any x were also calculated using the results obtained for the concentration. These values are given in Figures 6.1 through (6.8) for all the four cases analyzed. The comparison of these values with the experimental data shows good agreement with an average difference of about 1.39%, and a maximum of 2.67%.

Figure 6.1: Comparison of Vertical Concentration Profile.

y = 0 x = 100m

Run # 20 Prairie Grass

Present Method

Q_x = 101.7 g/s

Q(1)= 101.2 g/s

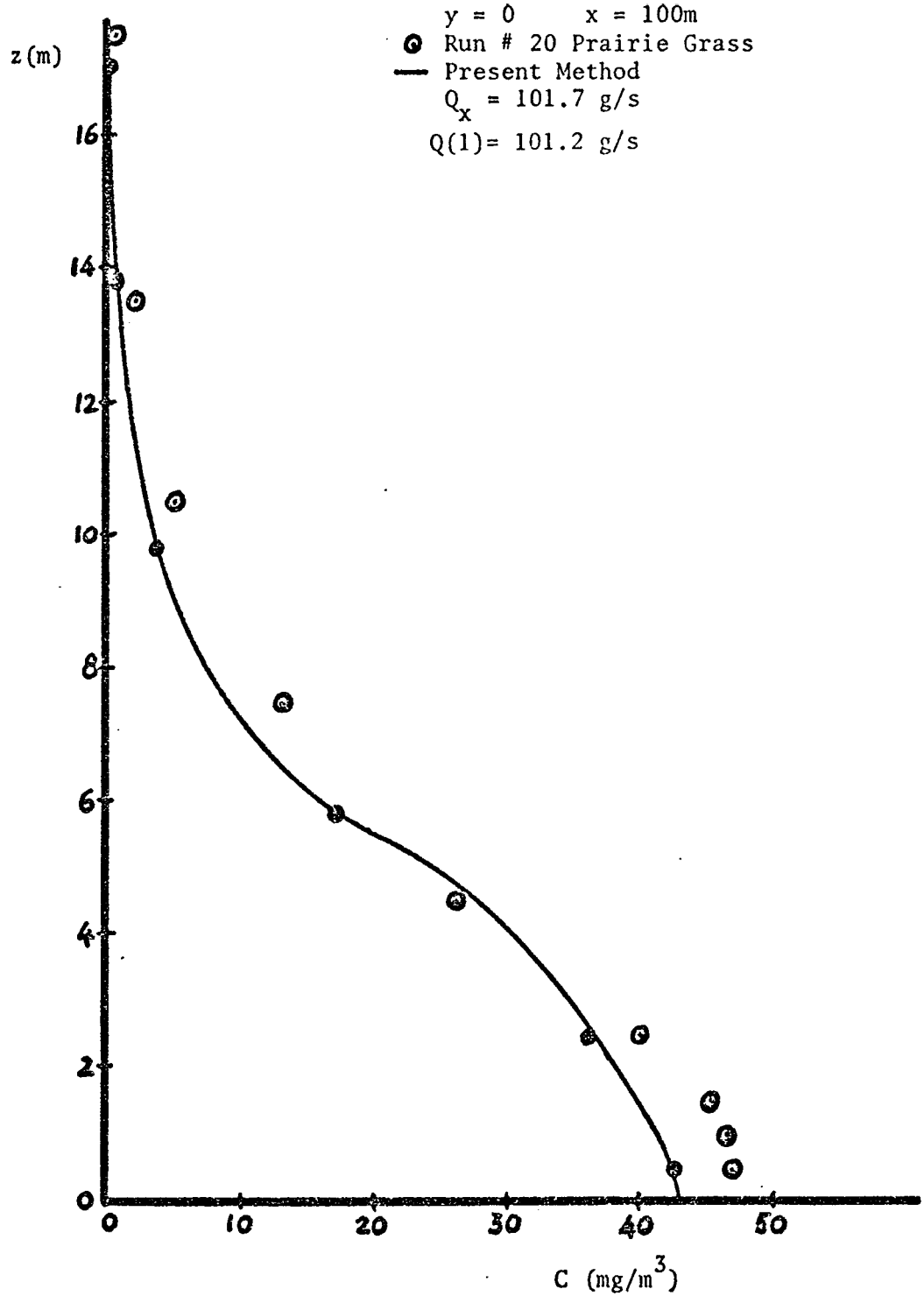


Figure 6.2: Comparison of Vertical Concentration Profile.
y = 0 x = 100m
⊙ Run # 24 Prairie Grass
— Present Method
Q_x = 41.7 g/s
Q(1)= 41.2 g/s

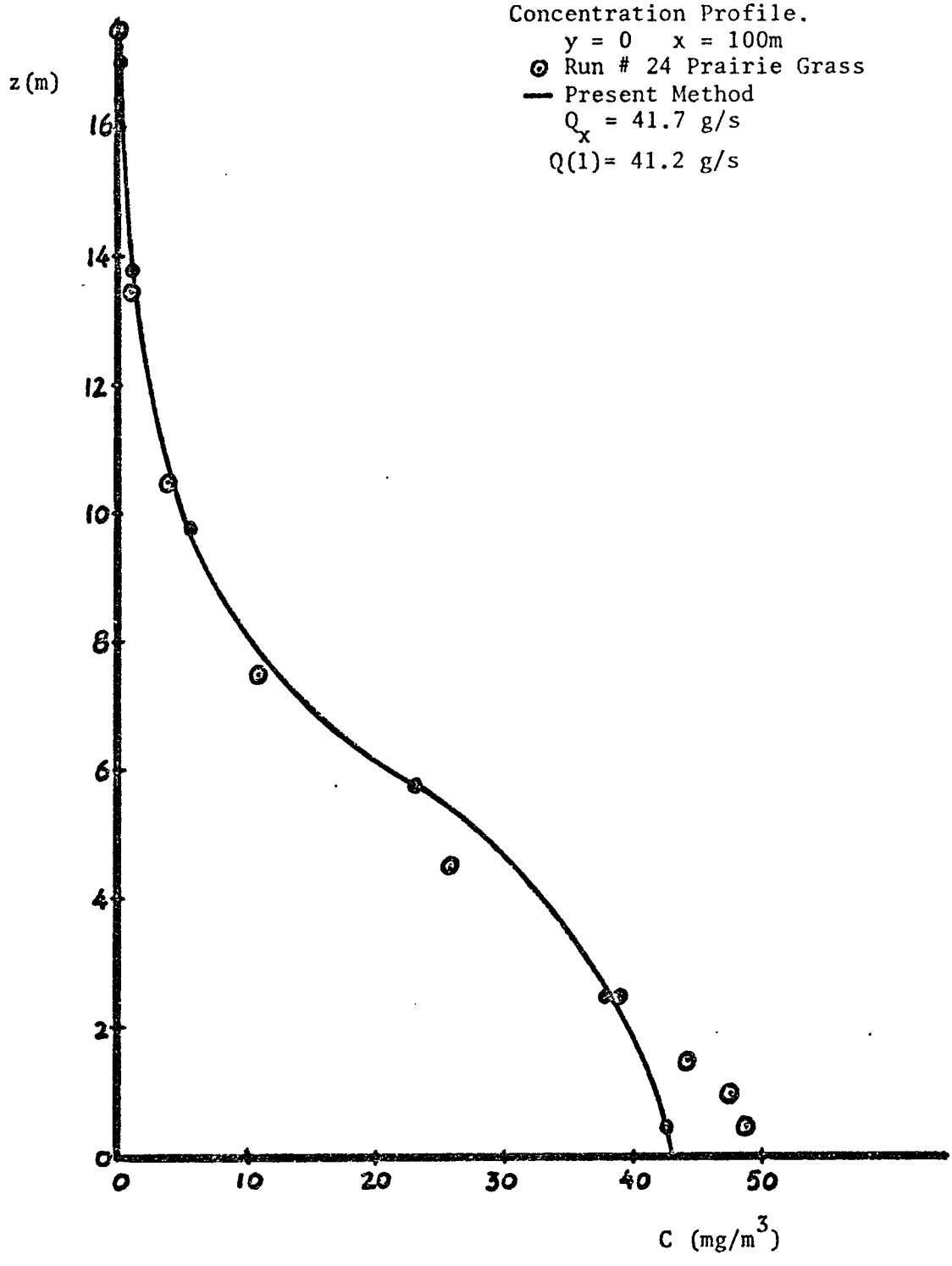


Figure 6.3: Comparison of Vertical Concentration Profile.
y = 0 x = 100m
Run # 45 Prairie Grass
--- Bullin' Method
— Present Method
Q_x = 101.3 g/s
Q(1) = 100.8 g/s

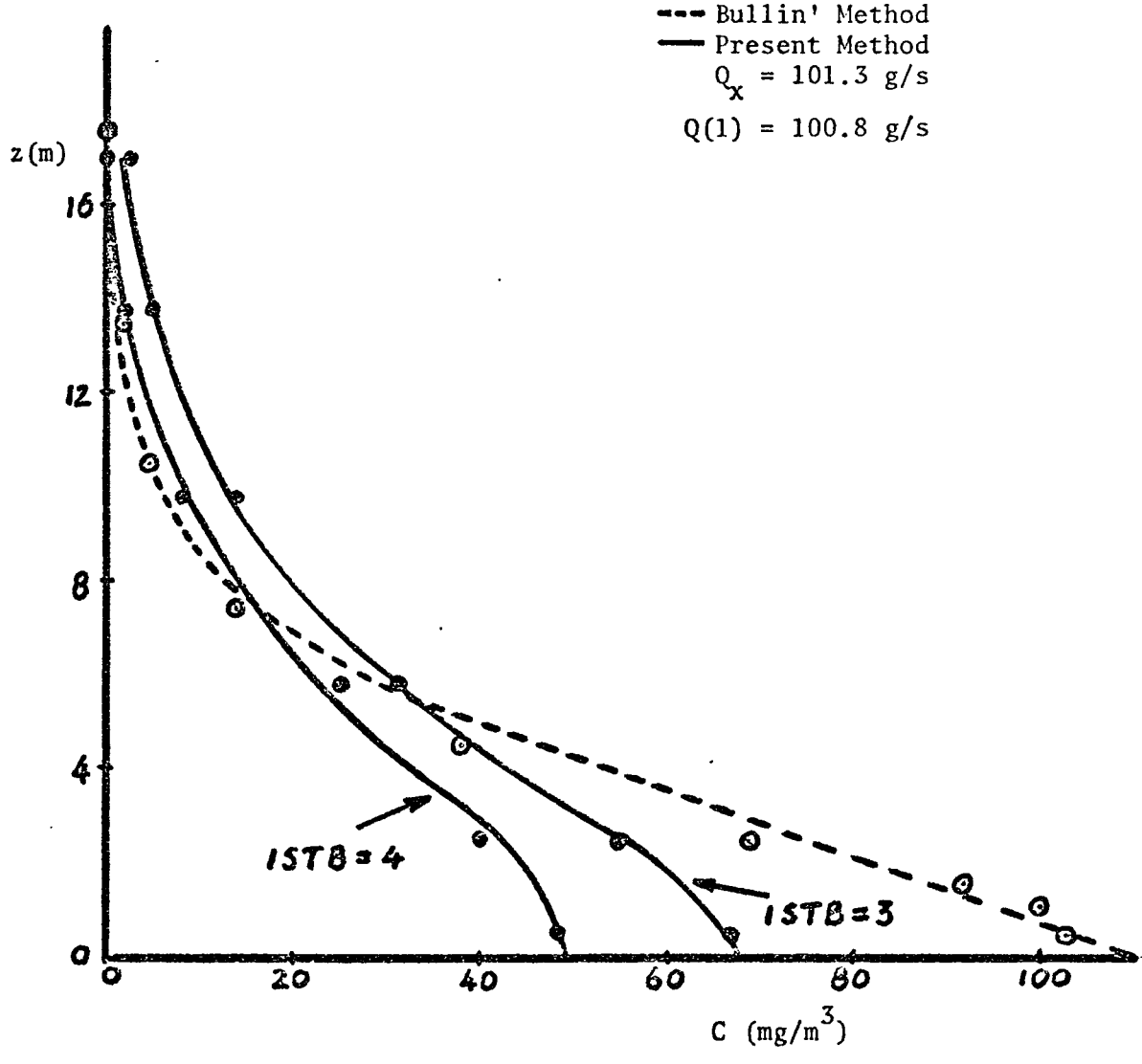


Figure 6.4: Comparison of Vertical Concentration Profile.
y = 0 x = 100m
Run # 54 Prairie Grass
Bullin' Method
Present Method
Q_x = 44.4 g/s
Q(1) = 43.4 g/s

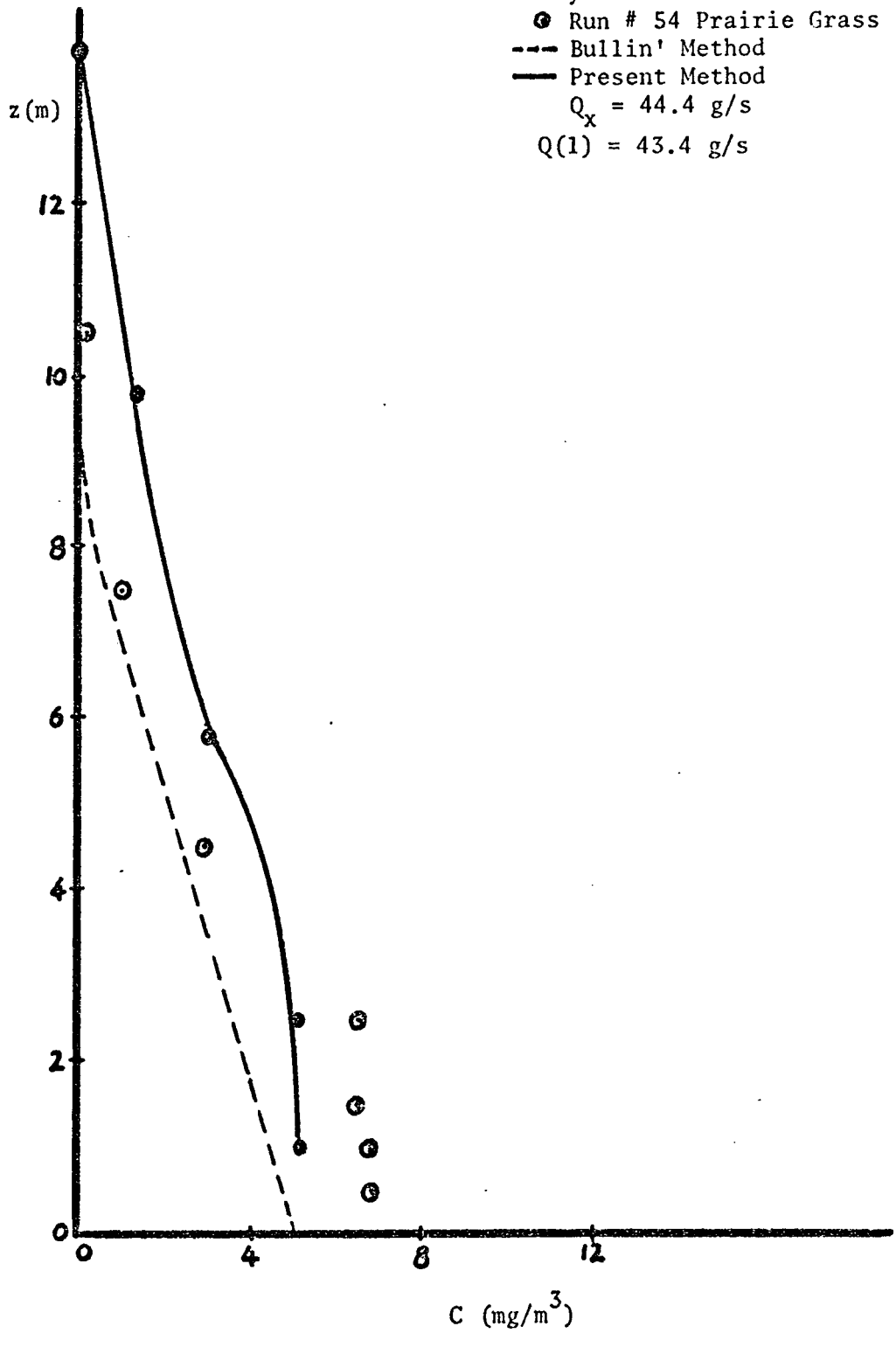
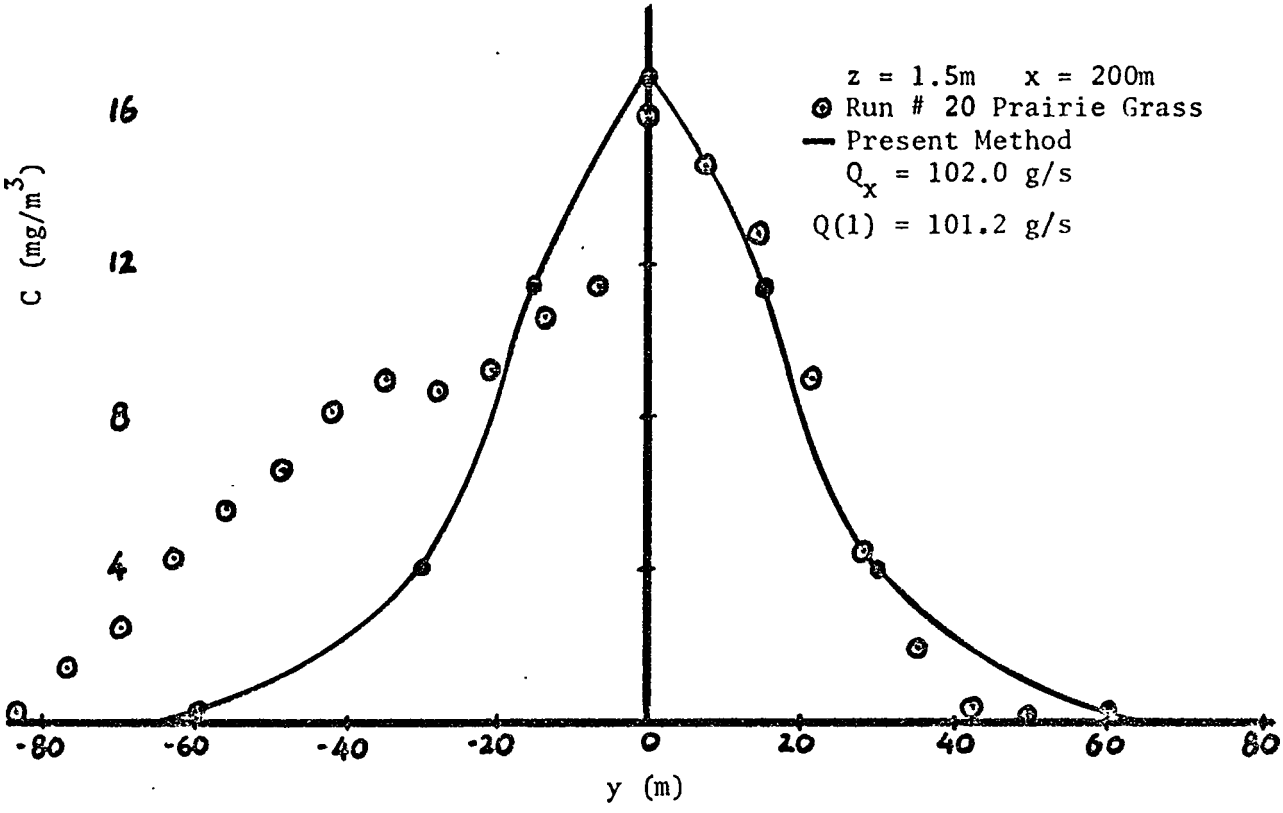


Figure 6.5: Comparison of Horizontal Concentration Profile.



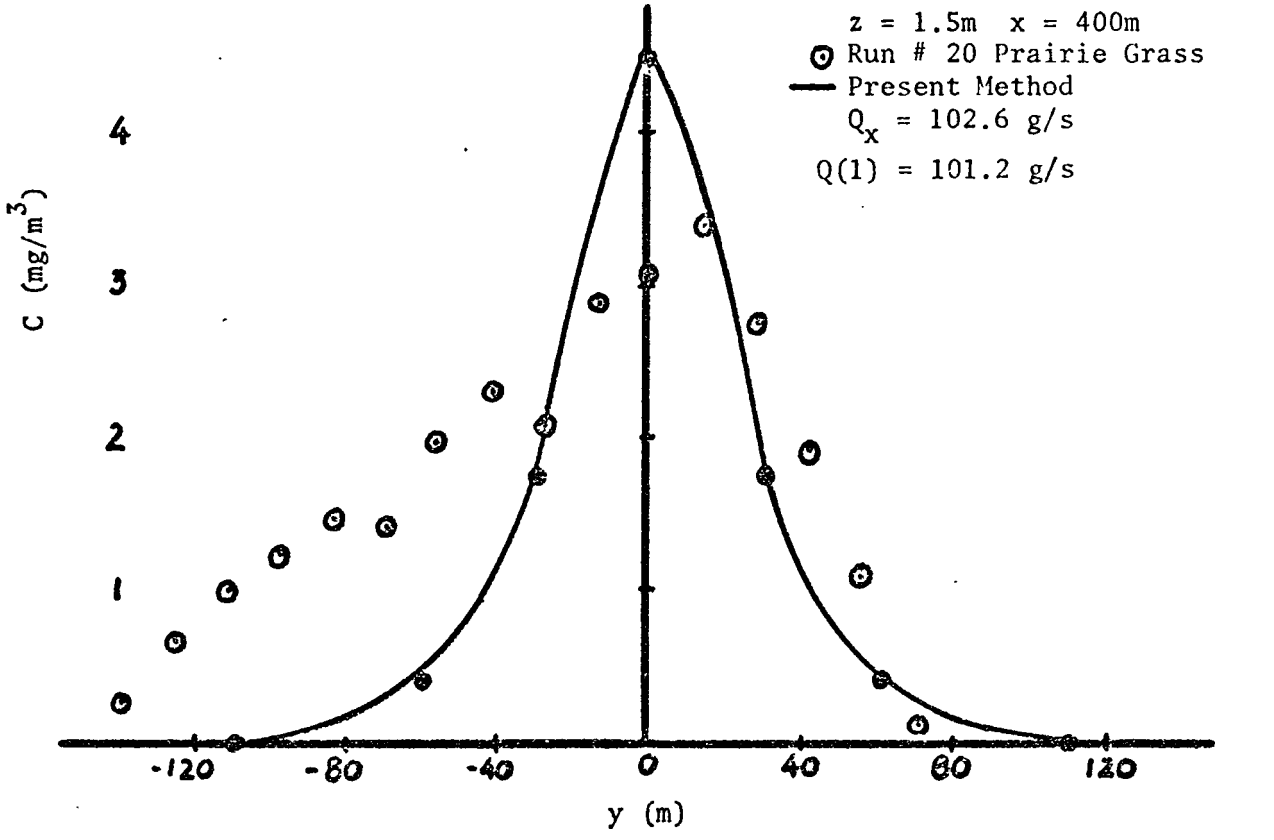
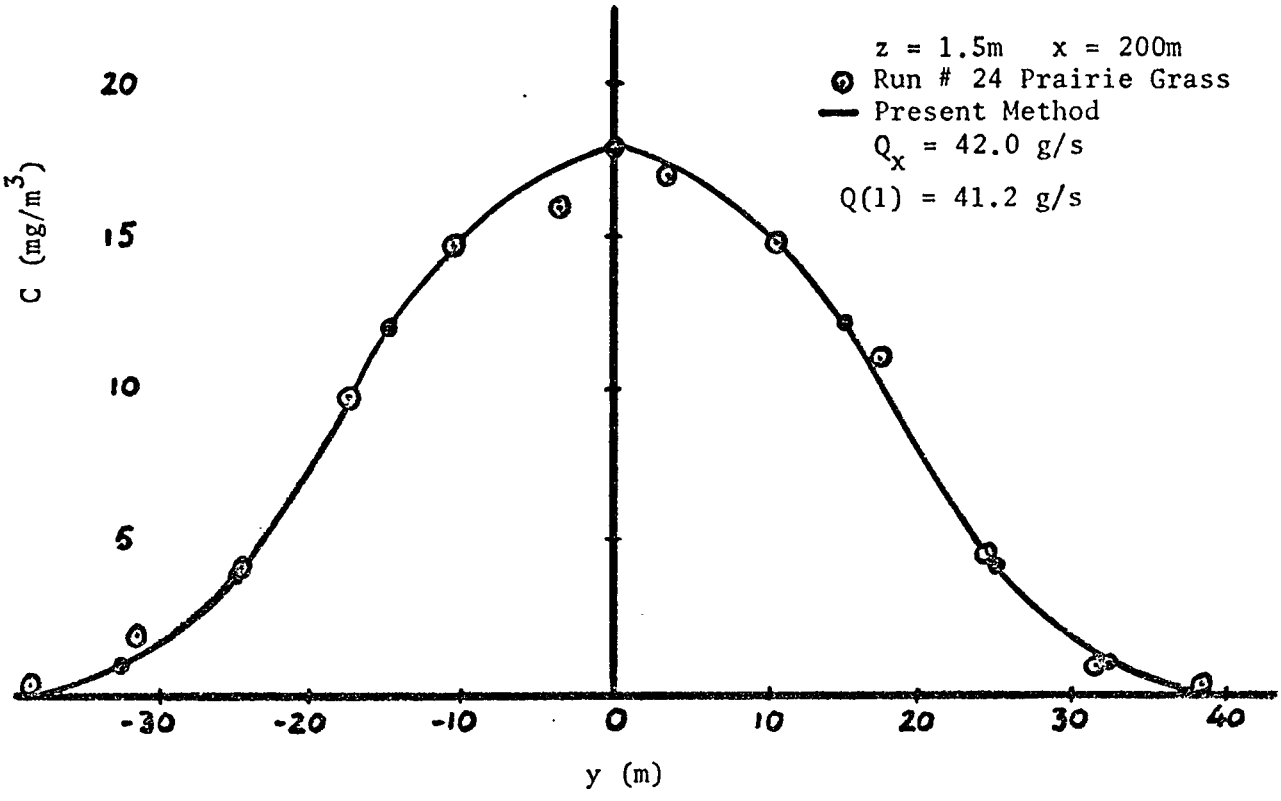


Figure 6.6: Comparison of Horizontal Concentration Profile.



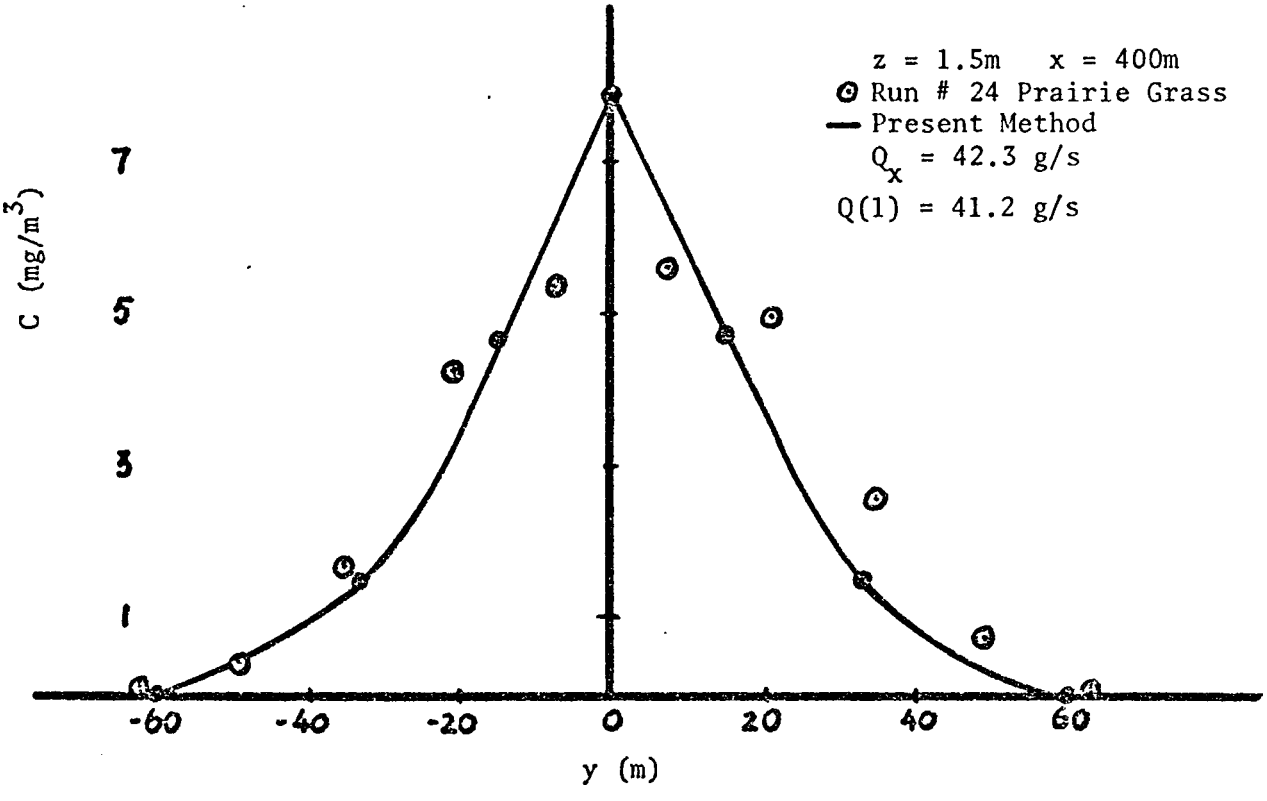
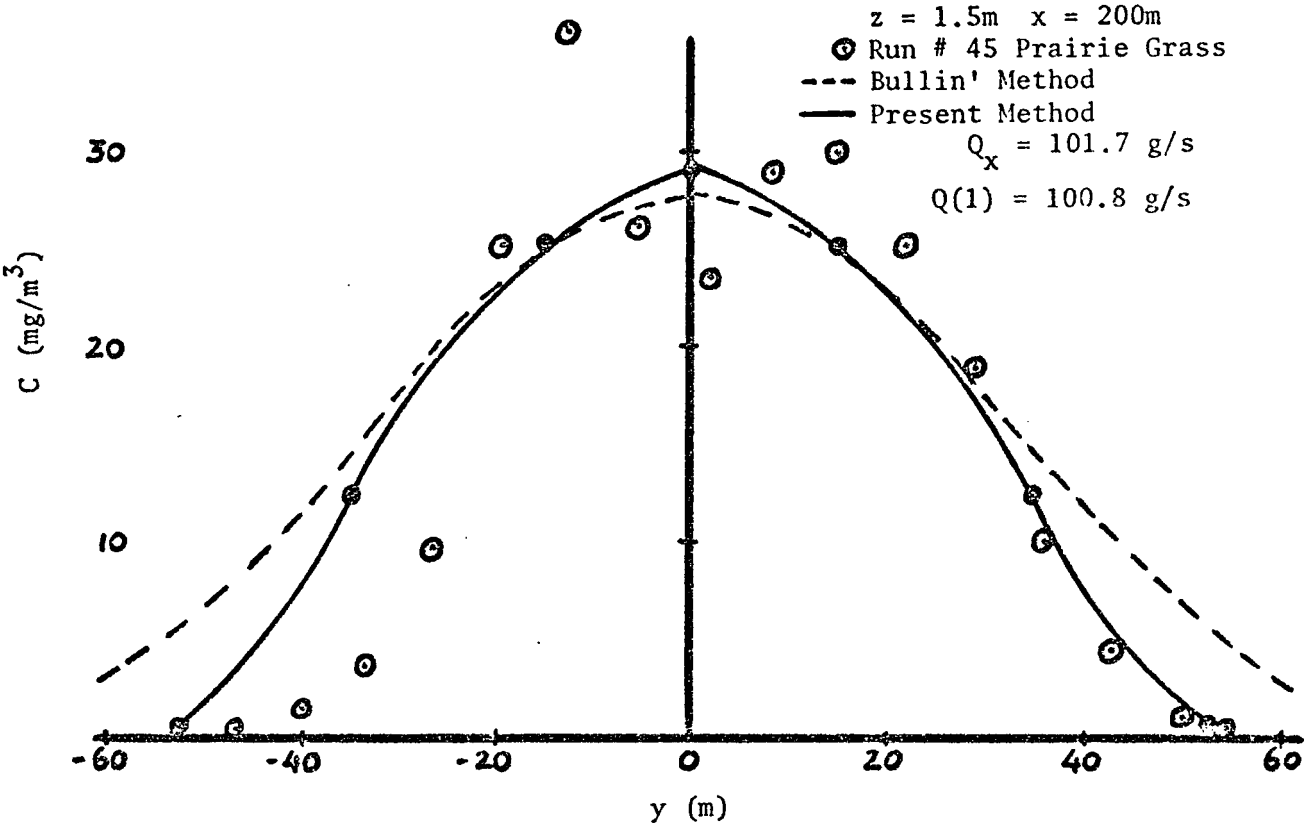


Figure 6.7: Comparison of Horizontal Concentration Profile.



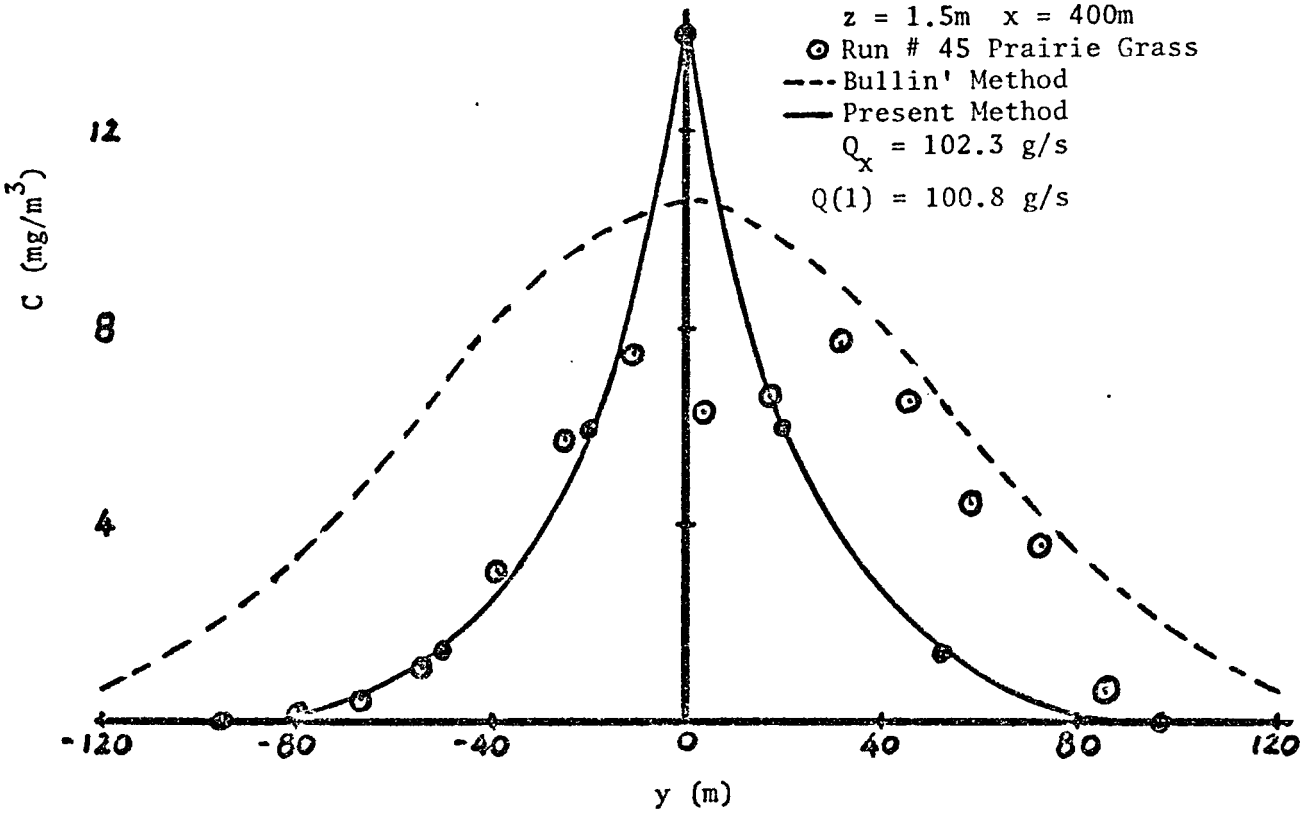
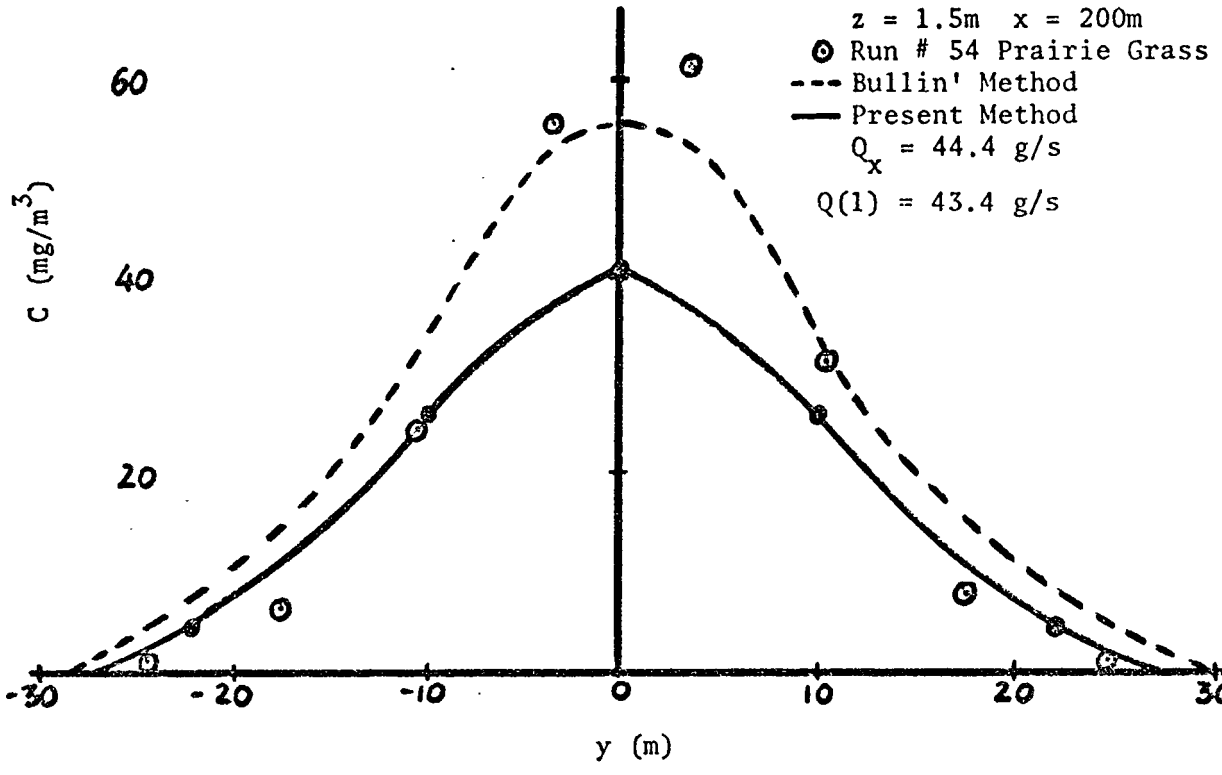
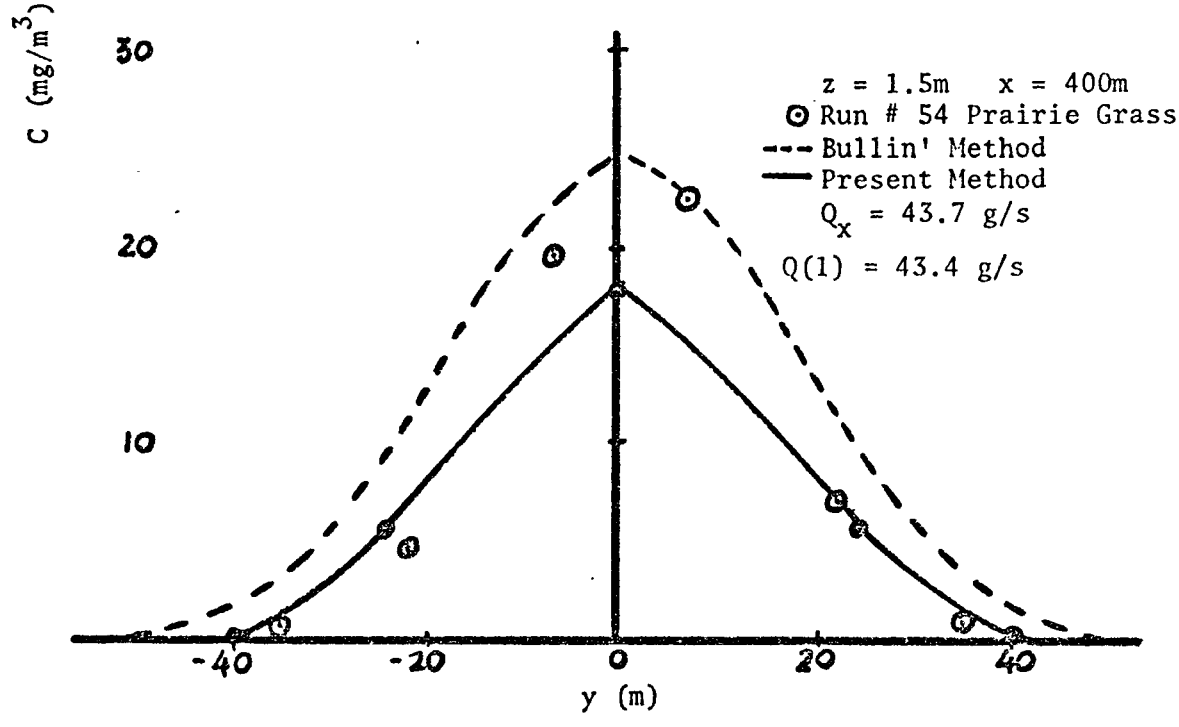


Figure 6.8: Comparison of Horizontal Concentration Profile.





Hypothetical Cases

Concentration profiles were simulated for all the hypothetical cases shown in Table 6.3. Vertical profiles at the centerline (y=0) and at several downwind locations for cases 4 through 6 are shown as a function of time in Figures 6.9 through 6.12. As it would be expected, there is a peak in the concentration at the elevation of the effective emission height. The value of this concentration peak increases as the atmospheric stability increases.

The concentration distribution for cases 1 through 7, at the steady state and for different x and y locations are shown in Tables 6.4 and 6.5. These correspond to an elevation of the effective emission height and the ground level, respectively.

Tables 6.6 and 6.7 show case 8, where a velocity in the y direction is included. This case is explained as a function of time so that the development of the plume can be clearly visualized.

This parametric study, i.e., cases 1 through 8, will be analyzed in more detail in the next section.

A multiple source case is shown in Table 6.9, and each source acting individually is shown in Table 6.8. The effect of their interaction can be obtained by comparing both Tables.

Table 6.3 : Hypothetical Cases Simulated

CASE	NO. OF SOURCES	SOURCE LOCATION (m)[1]	SOURCE STRENGTH (kg/s)	STABILITY CLASS[2]	ALPHA	UST (m/s)	RATE OF REACTION (min^{-1})[3]	AM	P(%)
1	1	(0,0,150)	5	D	1	5	0	.25	0
2	1	(0,0,150)	5	D	2	5	0	.15	0
3	1	(0,0,150)	5	D	2	5	0	.25	0
4	1	(0,0,150)	5	D	2	5	5.8×10^{-5}	.25	0
5	1	(0,0,150)	5	B	2	5	5.8×10^{-5}	.25	0
6	1	(0,0,150)	5	E	2	5	5.8×10^{-5}	.25	0
7	1	(0,0,252.5)	5	D	2	5	5.8×10^{-5}	.25	0
8	1	(0,0,150)	5	D	2	5	5.8×10^{-5}	.25	5
9	1	(0,-284.1, 252.5)	3	D	2	5	5.8×10^{-5}	.25	0
10	2	(0,0,150)	5	D	2	5	5.8×10^{-5}	.25	0
		(10000,-284.1, 252.5)	3	D	2	5	5.8×10^{-5}	.25	0

(1) The value in the z direction refers to the effective emission height.

(2) Using Pasquill-Gifford definition for stability categories.

(3) Rate of reaction for a first-order reaction.

It should be noted that the concentration distribution due to each source acting individually is at the steady state. This occurs when the time between the start of release and the initiation of the averaging time, Θ, is equal to 80 minutes and the end of the averaging time, Ω, is equal to 90 minutes. However, when both sources are put together, the steady state is reached after a longer time.

For all of the cases simulated without reaction, the differences between the mass flux at any x location, at steady state, and the constant source emission rate were not more than 4% of the emission rate. These results show the validity of the model in computing the concentration distribution, and also that the present method can handle continuity calculations.

Figure 6.9: Vertical Concentration Profiles for
Hypothetical Cases 4, 5 and 6.

Θ = 0 min
Ω = 10 min
y = 0

..... Stability Class B
– – – Stability Class D
——— Stability Class E

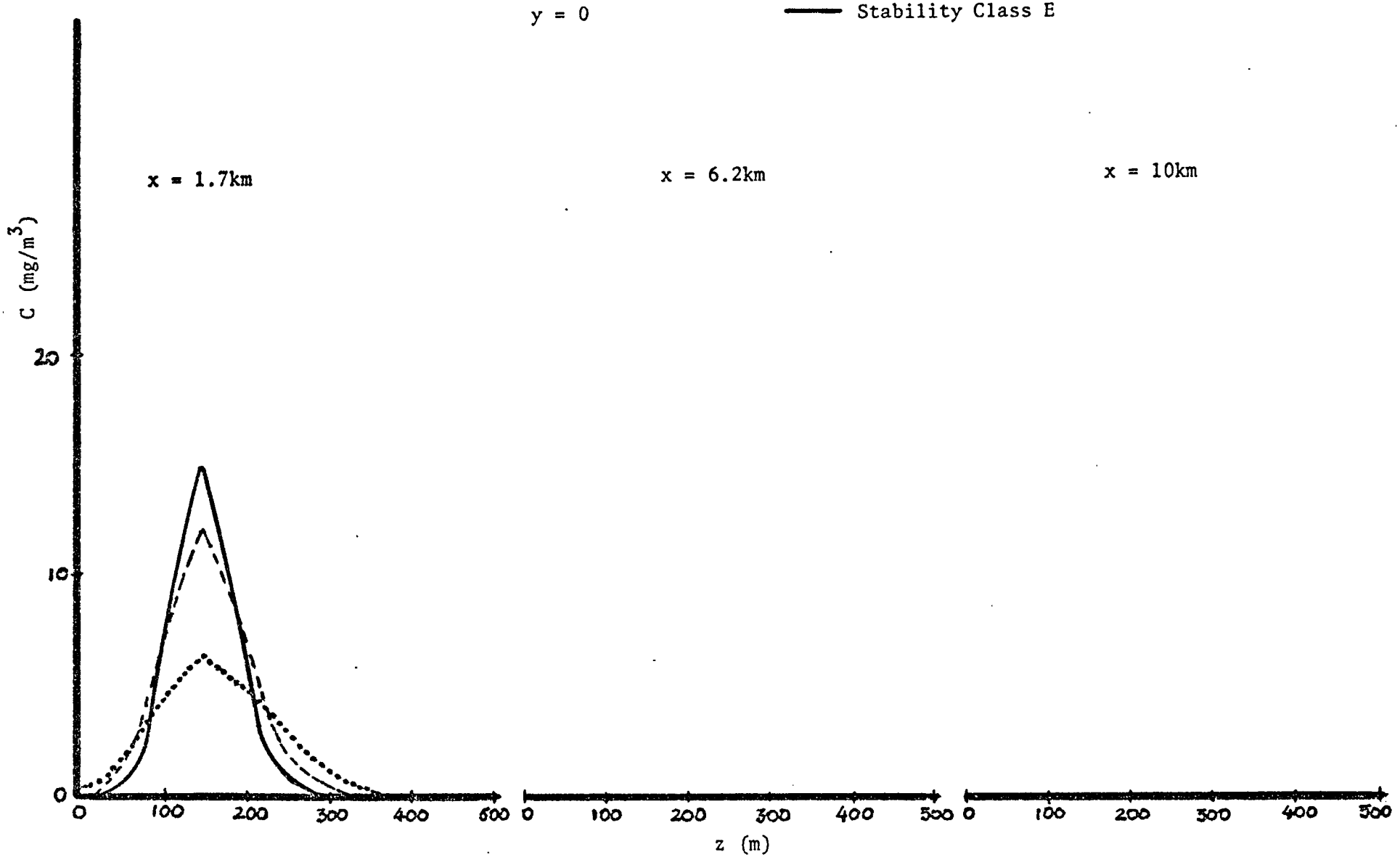


Figure 6.10: Vertical Concentration Profiles for
Hypothetical Cases 4, 5 and 6.

Θ = 20 min ..... Stability Class B
Ω = 30 min – – – Stability Class D
y = 0 ——— Stability Class E

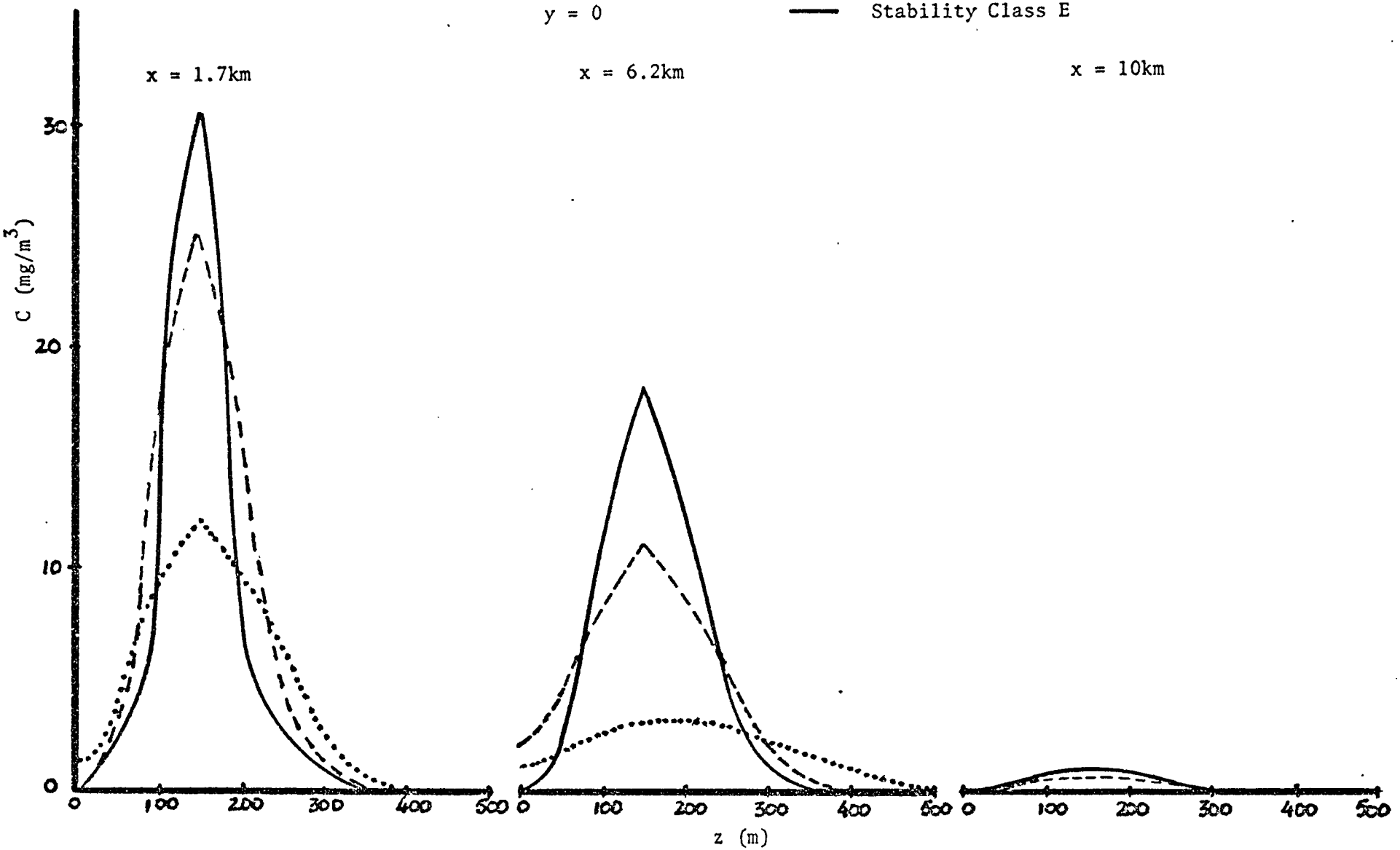


Figure 6.11: Vertical Concentration Profiles for Hypothetical Cases 4, 5 and 6.

Θ = 35 min
Ω = 45 min
y = 0

..... Stability Class B
– – – Stability Class D
——— Stability Class E

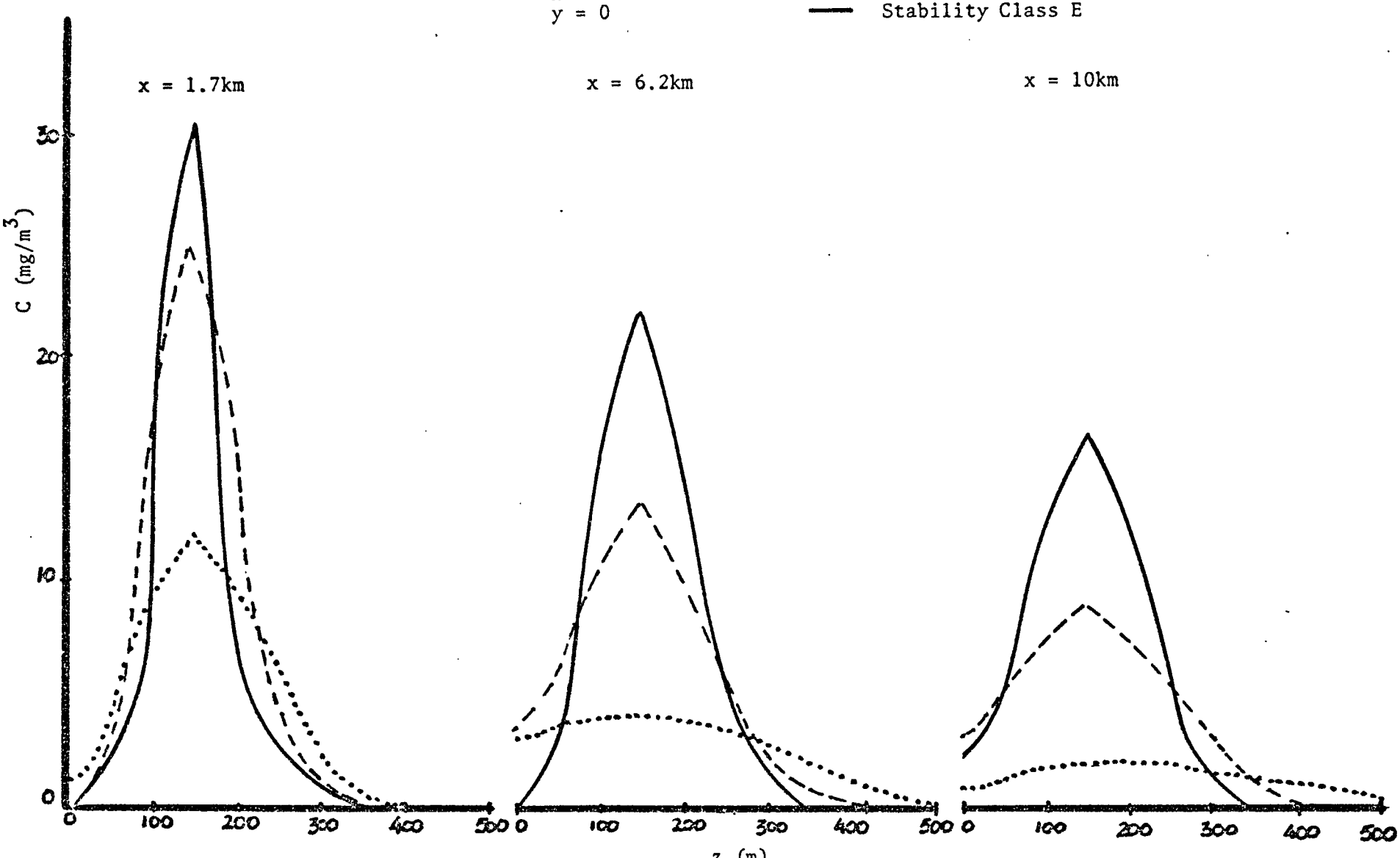


Figure 6.12: Vertical Concentration Profiles for Hypothetical Cases 4, 5 and 6.

Θ = 80 min
Ω = 90 min
y = 0

····· Stability Class B
– – – Stability Class D
——— Stability Class E

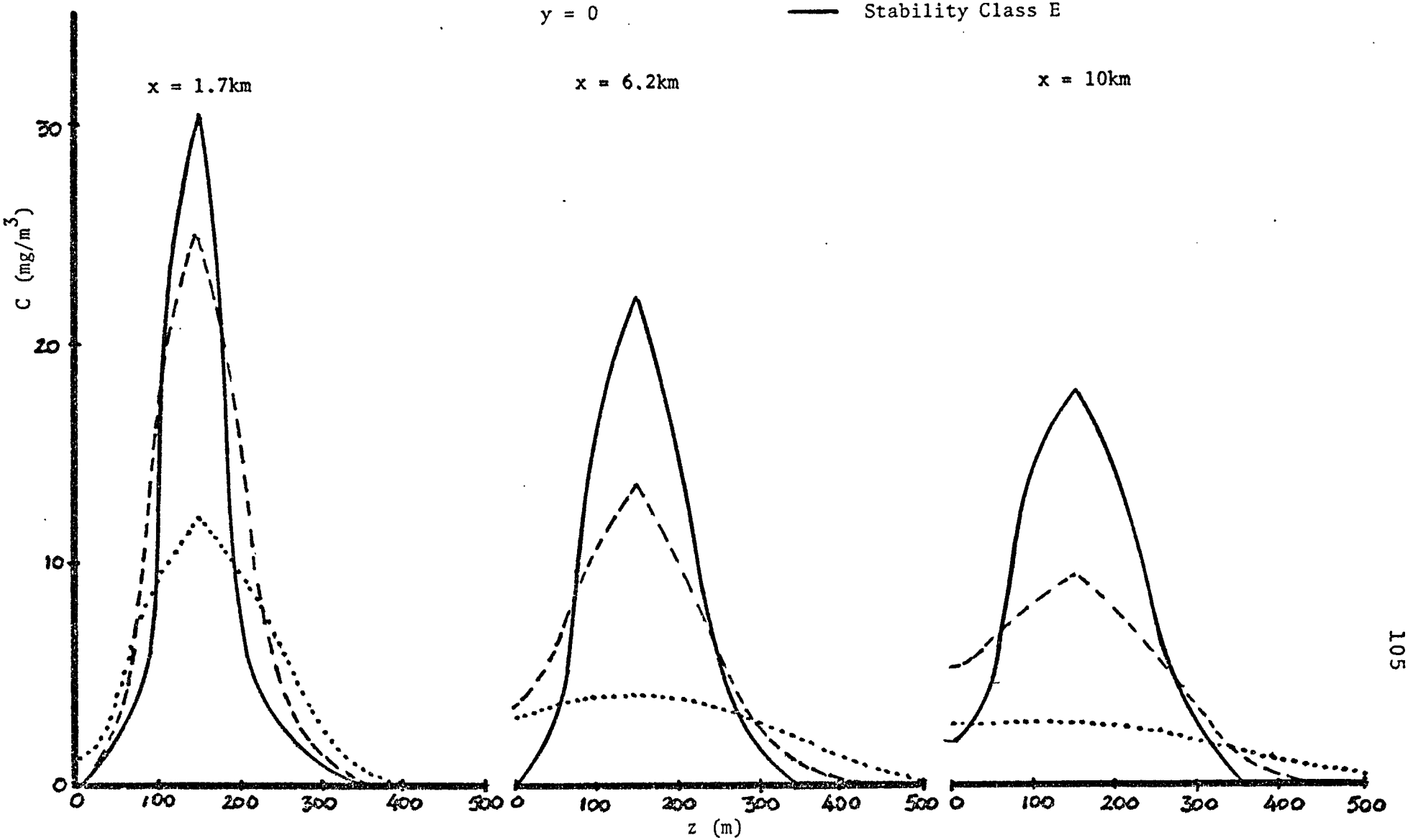


Table 6.4 Concentration Distribution for Hypothetical Cases 1 Through 7 (θ = 80 min, Ω = 90 min)

X DIRECTION (METERS)

	0.0	337.7	1694.0	3806.9	6193.1	8306.0	9662.3	10000.0	
				CONCENTRATION (MG/CU.M)					
				**********					
Z DIRECTION =	150.0 M								
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.16	0.61	1.00	1.24	1.37	1.44	1.45	Case #1
Y= 0.0 M	35.45	33.11	26.06	19.48	15.15	12.72	11.57	11.32	
Y= 284.1 M	0.0	0.16	0.61	1.00	1.24	1.37	1.44	1.45	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.28	2.28	Case #2
Y= 0.0 M	35.45	32.88	25.22	18.18	13.63	11.11	9.92	9.67	
Y= 284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.28	2.28	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.31	1.16	1.81	2.12	2.25	2.29	2.30	Case #3
Y= 0.0 M	35.45	32.89	25.22	18.19	13.65	11.14	9.96	9.71	
Y= 284.1 M	0.0	0.31	1.16	1.81	2.12	2.25	2.29	2.30	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.29	2.29	
Y= 0.0 M	35.45	32.88	25.22	18.18	13.63	11.12	9.94	9.69	
Y= 284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.29	2.29	Case #4
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.10	0.41	1.34	1.80	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.28	0.41	0.33	0.27	
Y=-284.1 M	0.0	0.95	2.13	2.11	1.96	1.81	1.78	1.78	
Y= 0.0 M	35.45	26.93	12.15	6.44	3.98	3.19	2.72	2.64	Case #5
Y= 284.1 M	0.0	0.95	2.13	2.11	1.96	1.81	1.78	1.78	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.28	0.41	0.33	0.27	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.10	0.41	1.34	1.80	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.13	0.58	1.08	1.47	1.70	1.82	1.85	
Y= 0.0 M	35.45	34.38	30.61	26.02	22.13	19.48	18.06	17.74	Case #6
Y= 284.1 M	0.0	0.13	0.58	1.08	1.47	1.70	1.82	1.85	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.01	0.18	0.57	0.95	1.21	1.33	1.36	Case #7
Y= 0.0 M	0.0	1.08	3.91	5.70	6.14	6.00	5.81	5.76	
Y= 284.1 M	0.0	0.01	0.18	0.57	0.95	1.21	1.33	1.36	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Z DIRECTION =	252.5 M								
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.29	1.11	1.77	2.11	2.24	2.28	2.29	
Y= 0.0 M	32.39	30.35	24.00	17.79	13.56	11.13	9.96	9.70	Case #7
Y= 284.1 M	0.0	0.29	1.11	1.77	2.11	2.24	2.28	2.29	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Table 6.5 Concentration Distribution for Hypothetical Cases 1 Through 7 (θ = 80 min, Ω = 90 min)

X DIRECTION (METERS)

0.0 337.7 1694.0 3806.9 6193.1 8306.0 9662.3 10000.0

CONCENTRATION(MG/CU.M)
****

Z DIRECTION = 0.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.09	0.38	0.68	0.87	0.91	
Y= 0.0 M	0.0	0.0	0.0	1.59	4.03	5.48	6.08	6.20	Case #1
Y= 284.1 M	0.0	0.0	0.0	0.09	0.38	0.68	0.87	0.91	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.12	0.52	0.92	1.16	1.22	Case #2
Y= 0.0 M	0.0	0.0	0.0	1.18	3.13	4.25	4.70	4.79	
Y= 284.1 M	0.0	0.0	0.0	0.12	0.52	0.92	1.16	1.22	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	Case #3
Y= 0.0 M	0.0	0.0	0.0	1.48	3.59	4.72	5.15	5.23	
Y= 284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	Case #4
Y= 0.0 M	0.0	0.0	0.0	1.48	3.58	4.72	5.14	5.22	
Y= 284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.08	0.04	0.05	0.05	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.38	0.54	0.54	0.52	
Y=-284.1 M	0.0	0.0	0.27	1.18	1.64	1.75	1.76	1.77	Case #5
Y= 0.0 M	0.0	0.0	1.10	3.03	2.93	2.80	2.55	2.52	
Y= 284.1 M	0.0	0.0	0.27	1.18	1.64	1.75	1.76	1.77	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.38	0.54	0.54	0.52	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.08	0.04	0.05	0.05	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.02	0.13	0.22	0.24	
Y= 0.0 M	0.0	0.0	0.0	0.0	0.35	1.44	2.14	2.31	Case #6
Y= 284.1 M	0.0	0.0	0.0	0.0	0.02	0.13	0.22	0.24	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.02	0.08	0.14	0.16	Case #7
Y= 0.0 M	0.0	0.0	0.0	0.0	0.05	0.34	0.56	0.62	
Y= 284.1 M	0.0	0.0	0.0	0.0	0.02	0.08	0.14	0.16	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Table 6.6 Concentration Distribution for Hypothetical Case #8

X DIRECTION (METERS)

0.0	337.7	1694.0	3806.9	6193.1	8306.0	9662.3	10000.0

CONCENTRATION(MG/CU.M)

Z DIRECTION = 150.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 0.0 M	35.45	22.36	11.81	1.08	0.0	0.0	0.0	0.0	Θ = 0 min
Y= 284.1 M	0.0	0.88	1.93	0.34	0.0	0.0	0.0	0.0	Ω = 10 min
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 5 min
Y= 0.0 M	35.45	33.13	19.83	5.07	0.0	0.0	0.0	0.0	Ω = 15 min
Y= 284.1 M	0.0	1.53	4.78	2.84	0.0	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 10 min
Y= 0.0 M	35.45	32.60	23.57	9.19	1.23	0.0	0.0	0.0	Ω = 20 min
Y= 284.1 M	0.0	1.95	7.64	7.40	1.72	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.12	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 20 min
Y= 0.0 M	35.45	32.77	22.15	10.86	3.87	0.79	0.16	0.08	Ω = 30 min
Y= 284.1 M	0.0	2.33	9.60	14.26	9.88	3.30	0.82	0.45	
Y= 519.1 M	0.0	0.0	0.0	0.04	3.29	2.05	0.59	0.33	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.21	0.14	0.09	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 0.0 M	35.45	32.71	22.29	9.92	2.65	0.0	0.0	0.0	Θ = 40 min
Y= 284.1 M	0.0	2.29	9.71	14.60	12.15	0.0	0.0	0.0	Ω = 50 min
Y= 519.1 M	0.0	0.0	0.0	0.12	6.76	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 0.0 M	35.45	32.71	22.28	9.92	2.64	0.0	0.0	0.0	Θ = 80 min
Y= 284.1 M	0.0	2.28	9.73	14.57	12.21	0.0	0.0	0.0	Ω = 90 min
Y= 519.1 M	0.0	0.0	0.0	0.10	6.79	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Table 6.7 Concentration Distribution for Hypothetical Case #8

X DIRECTION (METERS)

	0.0	337.7	1694.0	3806.9	6193.1	8306.0	9662.3	10000.0	
CONCENTRATION (MG/CU.M)									
Z DIRECTION = 0.0 M									
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 0 min
Y= 0.0 M	0.0	0.0	0.0	0.06	0.0	0.0	0.0	0.0	Ω = 10 min
Y= 284.1 M	0.0	0.0	0.0	0.01	0.0	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 5 min
Y= 0.0 M	0.0	0.0	0.0	0.27	0.0	0.0	0.0	0.0	Ω = 15 min
Y= 284.1 M	0.0	0.0	0.0	0.11	0.0	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 10 min
Y= 0.0 M	0.0	0.0	0.0	0.63	0.13	0.0	0.0	0.0	Ω = 20 min
Y= 284.1 M	0.0	0.0	0.0	0.44	0.16	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 20 min
Y= 0.0 M	0.0	0.0	0.0	0.96	0.84	0.14	0.0	0.0	Ω = 30 min
Y= 284.1 M	0.0	0.04	0.0	1.21	1.84	0.47	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.06	0.49	0.26	0.01	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 40 min
Y= 0.0 M	0.0	0.0	0.0	0.80	0.74	0.0	0.0	0.0	Ω = 50 min
Y= 284.1 M	0.0	0.0	0.0	1.17	3.26	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.02	1.77	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	Θ = 80 min
Y= 0.0 M	0.0	0.0	0.0	0.80	0.73	0.0	0.0	0.0	Ω = 90 min
Y= 284.1 M	0.0	0.0	0.0	1.18	3.26	0.0	0.0	0.0	
Y= 519.1 M	0.0	0.0	0.0	0.03	1.76	0.0	0.0	0.0	
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Table 6.8 Concentration Distribution

Case #4 (Θ = 0 min) (Ω = 10 min) Case #9

	R DIRECTION (METERS)								R DIRECTION (METERS)							
	0.0	337.7	1694.0	3806.9	6193.1	8304.0	9662.3	10000.0	0.0	270.8	1355.2	3045.5	4954.5	6644.8	7729.9	8000.0
	CONCENTRATION (PG/CU.M)								CONCENTRATION (PG/CU.M)							
Z DIRECTION = 503.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 497.1 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 439.7 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 355.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.06	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.43	1.20	0.51	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.04	0.03	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 252.5 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.19	0.54	0.23	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.01	0.08	0.03	0.0	0.0	0.0	0.0	21.27	13.58	9.36	2.13	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.83	1.74	0.33	0.0	0.0	0.0	0.0	0.0	0.10	0.31	0.14	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.01	0.08	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 150.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.08	0.06	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.24	0.52	0.10	0.0	0.0	0.0	0.0	0.0	0.43	1.19	0.51	0.0	0.0	0.0	0.0
Y= 0.0 M	35.45	22.17	12.04	1.15	0.0	0.0	0.0	0.0	0.0	0.00	0.04	0.03	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.24	0.52	0.10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 65.3 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.02	0.12	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	1.19	2.58	0.41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.02	0.12	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 12.9 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.07	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 0.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.06	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GRAM/SEC) =	4999.76	3491.84	2400.56	295.98	0.0	0.0	0.0	0.0	2999.86	2044.21	1757.16	498.90	0.0	0.0	0.0	0.0

Table 6.8 Continuation

(Θ = 10 min)
(Ω = 20 min)

	X DIRECTION (METERS)								X DIRECTION (METERS)							
	0.0	337.7	1694.0	3806.9	6193.1	8306.0	9662.3	10000.0	0.0	270.1	1355.2	3045.5	4954.5	6644.8	7729.5	8000.0
	CONCENTRATION (PG/CU.M)								CONCENTRATION (PG/CU.M)							
Z DIRECTION = 505.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.00	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 492.1 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.00	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 439.7 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.03	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 355.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.14	0.36	0.28	0.07	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.55	2.26	2.87	1.55	0.30	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.02	0.0	0.0	0.0	0.0	0.01	0.08	0.22	0.12	0.04	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 252.5 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.25	1.01	1.32	0.75	0.15	0.0	0.0
Y=-284.1 M	0.0	0.01	0.19	0.37	0.13	0.0	0.0	0.0	21.27	20.01	16.73	10.75	4.08	0.65	0.0	0.0
Y= 0.0 M	0.0	1.03	4.00	3.80	0.91	0.0	0.0	0.0	0.0	0.13	0.58	0.80	0.47	0.10	0.0	0.0
Y= 284.1 M	0.0	0.01	0.19	0.37	0.13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 150.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.12	0.36	0.28	0.07	0.0	0.0
Y=-284.1 M	0.0	0.10	1.19	1.20	0.31	0.0	0.0	0.0	0.0	0.55	2.25	2.87	1.55	0.30	0.0	0.0
Y= 0.0 M	35.45	32.72	25.44	12.27	2.14	0.0	0.0	0.0	0.0	0.01	0.08	0.22	0.12	0.04	0.0	0.0
Y= 284.1 M	0.0	0.10	1.19	1.20	0.31	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 65.3 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0
Y=-284.1 M	0.0	0.01	0.29	0.49	0.15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04	0.03	0.0	0.0
Y= 0.0 M	0.0	1.73	5.99	4.96	1.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0
Y= 284.1 M	0.0	0.01	0.29	0.49	0.15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 12.9 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.09	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.90	0.24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.09	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 0.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.06	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.81	0.20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.06	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Q(GR/SEC)=	4999.74	5027.41	5216.04	3348.93	702.90	0.0	0.0	0.0	2999.86	3014.46	3183.22	2645.00	1240.97	231.19	0.0	0.0

Table 6.8 Continuation

(Θ = 20 min)
(Ω = 30 min)

	X DIRECTION (METERS)								X DIRECTION (METERS)							
	0.0	337.7	1694.0	3606.9	6193.1	8306.0	9662.3	10000.0	0.0	270.1	1355.2	3045.5	4954.5	6644.8	7725.9	8000.0
	CONCENTRATION (MG/CU.M)								CONCENTRATION (MG/CU.M)							
Z DIRECTION = 505.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.05	0.04	0.04	0.04
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 492.1 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.07	0.06	0.05	0.05
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 439.7 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.08	0.07	0.07
Y=-284.1 M	0.0	0.0	0.0	0.0	0.01	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.12	0.32	0.28	0.28
Y= 0.0 M	0.0	0.0	0.0	0.0	0.07	0.02	0.01	0.01	0.0	0.0	0.0	0.0	0.01	0.05	0.05	0.05
Y= 284.1 M	0.0	0.0	0.0	0.0	0.01	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 385.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.72	0.66	0.47	0.41
Y=-284.1 M	0.0	0.0	0.0	0.0	0.04	0.05	0.02	0.01	0.0	0.58	2.20	3.42	3.75	2.77	1.35	1.15
Y= 0.0 M	0.0	0.0	0.0	0.0	0.25	0.26	0.10	0.06	0.0	0.00	0.08	0.26	0.46	0.43	0.31	0.27
Y= 284.1 M	0.0	0.0	0.0	0.0	0.04	0.05	0.02	0.01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 252.5 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.26	0.98	1.57	1.84	1.41	0.92	0.80
Y=-284.1 M	0.0	0.02	0.17	0.59	0.76	0.39	0.12	0.07	21.27	20.16	16.45	12.67	9.74	5.88	3.44	2.90
Y= 0.0 M	0.0	1.11	3.84	5.85	4.96	2.00	0.55	0.32	0.0	0.14	0.56	0.95	1.17	0.92	0.61	0.53
Y= 284.1 M	0.0	0.02	0.17	0.59	0.76	0.39	0.12	0.07	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 150.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.72	0.67	0.47	0.41
Y=-284.1 M	0.0	0.22	1.14	1.86	1.71	0.73	0.21	0.12	0.0	0.58	2.19	3.41	3.79	2.77	1.76	1.51
Y= 0.0 M	35.45	32.97	25.06	18.50	11.05	3.74	0.94	0.52	0.0	0.00	0.08	0.26	0.46	0.43	0.31	0.26
Y= 284.1 M	0.0	0.22	1.14	1.86	1.71	0.73	0.21	0.12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 45.3 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.09	0.08	0.08
Y=-284.1 M	0.0	0.03	0.25	0.80	0.93	0.41	0.10	0.05	0.0	0.0	0.0	0.0	0.16	0.36	0.30	0.27
Y= 0.0 M	0.0	1.86	5.75	7.81	5.96	2.06	0.45	0.20	0.0	0.0	0.0	0.0	0.02	0.06	0.05	0.05
Y= 284.1 M	0.0	0.03	0.25	0.80	0.93	0.41	0.10	0.05	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 12.9 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.00	0.0	0.20	0.37	0.13	0.01	0.0	0.0	0.0	0.0	0.0	0.02	0.03	0.04	0.04
Y= 0.0 M	0.0	0.0	0.0	1.75	2.23	0.61	0.01	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.01	0.01
Y= 284.1 M	0.0	0.00	0.0	0.20	0.37	0.13	0.01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 0.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.00
Y=-284.1 M	0.0	0.01	0.0	0.18	0.35	0.11	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.01	0.01
Y= 0.0 M	0.0	0.0	0.0	1.61	2.05	0.52	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.00
Y= 284.1 M	0.0	0.01	0.0	0.18	0.35	0.11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Q(GCM/SEC)=	4999.76	5100.34	5087.10	5149.54	3894.23	1490.48	390.11	216.25	2999.86	3043.10	3119.47	3129.05	3022.61	2169.12	1382.05	1169.79

Table 6.8 Continuation

(Θ = 40 min)
(Ω = 50 min)

	R DIRECTION (METERS)								R DIRECTION (METERS)							
	0.0	337.7	1694.0	3806.9	6193.1	8306.0	9662.3	10000.0	0.0	270.1	1355.2	3045.5	4954.5	6644.8	7729.9	8000.0
	CONCENTRATION (MG/CU.M)								CONCENTRATION (PG/CU.F)							
Z DIRECTION = 505.0 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.05	0.06	0.09	0.11
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0	0.0	0.0	0.01	0.01	0.02	0.02
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 492.1 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.07	0.08	0.12	0.13
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.02	0.0	0.0	0.0	0.0	0.01	0.01	0.02	0.02
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 435.7 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.11	0.17	0.18
Y=-284.1 M	0.0	0.0	0.0	0.0	0.01	0.01	0.03	0.03	0.0	0.0	0.0	0.0	0.12	0.45	0.62	0.66
Y= 0.0 M	0.0	0.0	0.0	0.0	0.08	0.07	0.11	0.13	0.0	0.0	0.0	0.0	0.01	0.07	0.11	0.12
Y= 284.1 M	0.0	0.0	0.0	0.0	0.01	0.01	0.03	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 355.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.73	0.93	1.02	1.05
Y=-284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.27	0.29	0.0	0.57	2.20	3.40	3.84	3.85	3.77	3.75
Y= 0.0 M	0.0	0.0	0.0	0.0	0.31	0.85	1.16	1.21	0.0	0.00	0.26	0.46	0.61	0.68	0.70	
Y= 284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.27	0.29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 252.5 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.26	0.99	1.57	1.87	1.97	1.99	1.99
Y=-284.1 M	0.0	0.01	0.18	0.57	0.94	1.21	1.36	1.39	21.27	20.14	16.48	12.63	9.86	8.16	7.32	7.14
Y= 0.0 M	0.0	1.08	3.90	5.72	6.10	6.03	5.92	5.86	0.0	0.14	0.57	0.95	1.18	1.28	1.32	1.33
Y= 284.1 M	0.0	0.01	0.18	0.57	0.94	1.21	1.36	1.39	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 150.0 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.73	0.93	1.03	1.05
Y=-284.1 M	0.0	0.31	1.16	1.82	2.10	2.26	2.34	2.34	0.0	0.57	2.20	3.39	3.84	3.86	3.79	3.77
Y= 0.0 M	35.45	32.89	25.20	18.21	13.57	11.18	10.12	9.83	0.0	0.00	0.08	0.25	0.46	0.61	0.68	0.70
Y= 284.1 M	0.0	0.31	1.16	1.82	2.10	2.26	2.34	2.34	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 65.3 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04	0.13	0.20	0.22
Y=-284.1 M	0.0	0.02	0.27	0.77	1.21	1.57	1.72	1.72	0.0	0.0	0.0	0.0	0.17	0.54	0.72	0.77
Y= 0.0 M	0.0	1.81	5.85	7.61	7.67	7.53	7.21	7.02	0.0	0.0	0.0	0.0	0.02	0.09	0.13	0.14
Y= 284.1 M	0.0	0.02	0.27	0.77	1.21	1.57	1.72	1.72	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 12.9 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.03	0.04	0.04
Y=-284.1 M	0.0	0.0	0.0	0.17	0.65	1.12	1.22	1.23	0.0	0.0	0.0	0.0	0.05	0.11	0.15	0.16
Y= 0.0 M	0.0	0.0	0.0	1.60	3.74	4.90	4.78	4.55	0.0	0.0	0.0	0.0	0.01	0.02	0.04	0.04
Y= 284.1 M	0.0	0.0	0.0	0.17	0.65	1.12	1.22	1.23	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 0.0 F																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y=-284.1 M	0.0	0.0	0.0	0.15	0.63	1.10	1.20	1.17	0.0	0.0	0.0	0.0	0.02	0.08	0.16	0.18
Y= 0.0 M	0.0	0.0	0.0	1.46	3.59	4.78	4.64	4.44	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y= 284.1 M	0.0	0.0	0.0	0.15	0.63	1.10	1.20	1.17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

CASE/SEC= 4999.76 5074.32 5136.58 5039.74 4860.68 4858.25 4826.14 4773.88 2999.86 3039.09 3126.83 3114.64 3064.48 3024.42 2989.57 2994.58

Table 6.8 Continuation

(Θ = 80 min)
(Ω = 90 min)

	X DIRECTION (METERS)								X DIRECTION (METERS)							
	0.0	337.9	1694.8	3806.9	6193.1	8306.0	9662.3	10000.0	0.0	270.1	1355.2	3045.5	4954.5	6644.8	7729.9	8000.0
	CONCENTRATION (PC/CU.M)								CONCENTRATION (PC/CU.M)							
Z DIRECTION = 305.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.05	0.06	0.10	0.11
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0	0.0	0.0	0.01	0.01	0.02	0.02
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 492.1 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.07	0.08	0.12	0.13
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0	0.0	0.0	0.01	0.01	0.02	0.02
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 439.7 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.11	0.17	0.19
Y=-284.1 M	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.03	0.0	0.0	0.0	0.0	0.12	0.45	0.63	0.67
Y= 0.0 M	0.0	0.0	0.0	0.0	0.08	0.07	0.11	0.12	0.0	0.0	0.0	0.0	0.01	0.07	0.11	0.12
Y= 284.1 M	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 355.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.73	0.93	1.03	1.05
Y=-284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.26	0.28	0.0	0.57	2.20	3.41	3.84	3.86	3.79	3.73
Y= 0.0 M	0.0	0.0	0.0	0.0	0.32	0.86	1.12	1.18	0.0	0.00	0.00	0.26	0.46	0.61	0.68	0.70
Y= 284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.26	0.28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 252.5 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.26	0.99	1.57	1.86	1.97	2.00	2.00
Y=-284.1 M	0.0	0.01	0.18	0.57	0.95	1.21	1.33	1.36	21.27	20.14	16.48	12.63	9.85	8.18	7.25	7.17
Y= 0.0 M	0.0	1.08	3.71	5.70	6.14	6.00	5.81	5.76	0.0	0.14	0.57	0.95	1.18	1.29	1.33	1.34
Y= 284.1 M	0.0	0.01	0.18	0.57	0.95	1.21	1.33	1.36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 150.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.72	0.93	1.04	1.06
Y=-284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.29	2.29	0.0	0.57	2.19	3.39	3.86	3.87	3.81	3.78
Y= 0.0 M	35.45	32.88	25.22	18.18	13.63	11.12	9.94	9.69	0.0	0.00	0.08	0.26	0.46	0.61	0.69	0.71
Y= 284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.29	2.29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 65.3 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.13	0.20	0.22
Y=-284.1 M	0.0	0.02	0.27	0.76	1.22	1.55	1.72	1.76	0.0	0.0	0.0	0.0	0.17	0.54	0.73	0.77
Y= 0.0 M	0.0	1.80	5.86	7.59	7.72	7.44	7.23	7.17	0.0	0.0	0.0	0.0	0.02	0.09	0.13	0.15
Y= 284.1 M	0.0	0.02	0.27	0.76	1.22	1.55	1.72	1.76	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 12.9 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.03	0.04	0.04
Y=-284.1 M	0.0	0.0	0.0	0.17	0.65	1.10	1.35	1.41	0.0	0.0	0.0	0.0	0.05	0.11	0.19	0.22
Y= 0.0 M	0.0	0.0	0.0	1.62	3.74	4.84	5.24	5.31	0.0	0.0	0.0	0.0	0.01	0.02	0.04	0.05
Y= 284.1 M	0.0	0.0	0.0	0.17	0.65	1.10	1.35	1.41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Z DIRECTION = 0.0 M																
Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.03
Y=-284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	0.0	0.0	0.0	0.0	0.02	0.08	0.16	0.19
Y= 0.0 M	0.0	0.0	0.0	1.48	3.58	4.72	5.14	5.23	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y= 284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G(GM/SEC)=	4999.76	5070.20	5144.48	5025.23	4899.54	4824.38	4777.16	4765.98	2999.86	3039.57	3125.78	3119.05	3058.20	3031.57	3006.72	2999.80

Table 6.9 Concentration Distribution for Case #10 (Θ = 0 min, Ω = 10 min)

X DIRECTION (METERS)

	0.0	337.7	1694.0	3806.9	6193.1	8306.0	9662.3	10000.0	10270.1	11355.2	13045.5	14954.5	16644.8	17729.9	18000.0

CONCENTRATION(PG/CU.M)

Z DIRECTION = 505.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 492.1 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 439.7 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 355.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.08	0.06	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.43	1.20	0.51	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.04	0.03	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 252.5 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.19	0.54	0.23	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.01	0.08	0.04	0.0	0.0	0.0	21.27	13.58	9.36	2.13	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.83	1.74	0.33	0.0	0.0	0.0	0.0	0.10	0.31	0.14	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.01	0.08	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 150.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.06	0.06	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.24	0.52	0.10	0.0	0.0	0.0	0.0	0.43	1.19	0.51	0.0	0.0	0.0	0.0
Y= 0.0 M	35.45	22.39	12.04	1.15	0.0	0.0	0.0	0.0	0.00	0.04	0.03	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.24	0.52	0.10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 65.3 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.02	0.17	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	1.39	2.58	0.41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.02	0.12	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 12.9 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.07	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 0.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.06	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

CAEGR/SEC)=	4999.76	3491.64	2400.56	295.58	0.0	0.0	0.0	2999.86	2064.21	1757.16	498.90	0.0	0.0	0.0	0.0

Table 6.9 Continuation

(Θ = 10 min)
(Ω = 20 min)

X DIRECTION (METERS)

0.0 337.7 1694.0 3806.9 6193.1 8306.0 9662.3 10000.0 10270.1 11355.2 13045.5 14954.5 16644.8 17726.9 18000.0

CONCENTRATION (PC/CU.M)

Z DIRECTION = 5C5.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 492.1 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 439.7 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.03	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 355.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.0	0.02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 252.5 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.25	1.01	1.32	0.75	0.15	0.0	0.0
Y=-284.1 M	0.0	0.01	0.19	0.37	0.13	0.0	0.0	21.27	20.01	16.73	10.75	4.08	0.65	0.0	0.0
Y= 0.0 M	0.0	1.03	4.00	3.80	0.91	0.0	0.0	0.0	0.13	0.58	0.60	0.47	0.10	0.0	0.0
Y= 284.1 M	0.0	0.01	0.19	0.37	0.13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 150.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.36	0.28	0.07	0.0	0.0
Y=-284.1 M	0.0	0.30	1.19	1.20	0.31	0.0	0.0	0.0	0.55	2.25	2.47	1.55	0.30	0.0	0.0
Y= 0.0 M	35.45	32.72	25.44	12.27	2.14	0.0	0.0	0.0	0.01	0.08	0.22	0.18	0.04	0.0	0.0
Y= 284.1 M	0.0	0.30	1.19	1.20	0.31	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 65.3 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.0	0.0
Y=-284.1 M	0.0	0.01	0.29	0.49	0.15	0.0	0.0	0.0	0.0	0.0	0.0	0.04	0.03	0.0	0.0
Y= 0.0 M	0.0	1.73	5.99	4.96	1.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.01	0.29	0.49	0.15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 12.9 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.09	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.90	0.24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.09	0.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 0.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-284.1 M	0.0	0.0	0.0	0.08	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 0.0 M	0.0	0.0	0.0	0.81	0.20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 284.1 M	0.0	0.0	0.0	0.08	0.03	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

CHECK/SEC1= 4999.76 5027.41 5216.04 5348.53 702.90 0.0 0.0 2999.86 3014.46 3183.22 2649.00 1240.97 231.19 0.0 0.0

Table 6.9 Continuation

(Θ = 20 min)
(Ω = 30 min)

X DIRECTION (METERS)

0.0 337.7 1694.0 3806.9 6193.1 8306.0 9662.3 10000.0 10270.1 11355.2 13045.9 14954.5 16644.8 17725.9 18000.0

CONCENTRATION (PG/CU.M)

Z DIRECTION = 505.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.05	0.04	0.04	0.04
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 492.1 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.07	0.06	0.05	0.05
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.0	0.0	0.01	0.01	0.01	0.01
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 439.7 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.06	0.07	0.07
Y=-284.1 M	0.0	0.0	0.0	0.0	0.01	0.00	0.00	0.00	0.0	0.0	0.0	0.12	0.32	0.26	0.26
Y= 0.0 M	0.0	0.0	0.0	0.0	0.07	0.02	0.01	0.01	0.00	0.0	0.0	0.01	0.05	0.05	0.05
Y= 284.1 M	0.0	0.0	0.0	0.0	0.01	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 355.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.72	0.66	0.47	0.41
Y=-284.1 M	0.0	0.0	0.0	0.0	0.04	0.05	0.02	0.01	0.56	2.19	3.42	3.79	2.17	1.75	1.50
Y= 0.0 M	0.0	0.0	0.0	0.0	0.25	0.26	0.10	0.06	0.02	0.07	0.26	0.45	0.43	0.31	0.28
Y= 284.1 M	0.0	0.0	0.0	0.0	0.04	0.05	0.02	0.01	0.00	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 252.5 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.26	0.58	1.57	1.84	1.41	0.92	0.80
Y=-284.1 M	0.0	0.02	0.17	0.59	0.76	0.39	0.12	21.34	20.18	16.45	12.68	9.73	5.89	3.43	2.90
Y= 0.0 M	0.0	1.11	3.84	5.85	4.96	2.00	0.55	0.32	0.23	0.54	0.97	1.16	0.93	0.81	0.73
Y= 284.1 M	0.0	0.02	0.17	0.59	0.76	0.39	0.12	0.07	0.01	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 150.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.42	0.72	0.67	0.47	0.41
Y=-284.1 M	0.0	0.32	1.14	1.86	1.71	0.73	0.21	0.12	0.01	2.18	3.41	3.79	2.77	1.76	1.51
Y= 0.0 M	35.45	32.97	25.06	18.50	11.09	3.74	0.94	0.57	0.15	0.05	0.28	0.44	0.44	0.31	0.28
Y= 284.1 M	0.0	0.32	1.14	1.86	1.71	0.73	0.21	0.12	0.03	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 65.3 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.09	0.08	0.08
Y=-284.1 M	0.0	0.03	0.25	0.80	0.93	0.41	0.10	0.05	0.0	0.0	0.0	0.16	0.36	0.30	0.27
Y= 0.0 M	0.0	1.96	5.75	7.81	5.96	2.06	0.45	0.20	0.06	0.0	0.00	0.02	0.06	0.05	0.05
Y= 284.1 M	0.0	0.03	0.25	0.80	0.93	0.41	0.10	0.05	0.01	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 12.9 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.01
Y=-284.1 M	0.0	0.00	0.0	0.20	0.37	0.13	0.01	0.0	0.0	0.0	0.0	0.02	0.03	0.04	0.04
Y= 0.0 M	0.0	0.0	0.0	1.75	2.23	0.61	0.01	0.0	0.00	0.0	0.01	0.00	0.01	0.01	0.01
Y= 284.1 M	0.0	0.00	0.0	0.20	0.37	0.13	0.01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 0.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.01	0.01
Y=-284.1 M	0.0	0.01	0.0	0.18	0.35	0.11	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.03	0.03
Y= 0.0 M	0.0	0.0	0.0	1.61	2.05	0.52	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.01	0.00
Y= 284.1 M	0.0	0.01	0.0	0.18	0.35	0.11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

GMICR/SEC1= 4999.76 5100.34 5087.10 5149.54 3894.23 1490.48 990.11 3216.08 3102.40 3108.67 3135.00 3017.97 2172.17 1380.22 1192.69

Table 6.9 Continuation

(Θ = 40 min)
(Ω = 50 min)

X DIRECTION (METERS)

0.0 337.7 1694.0 3806.9 6193.1 8306.0 9662.3 10000.0 10270.1 11355.2 13045.5 14954.5 16644.8 17725.9 18000.0

CONCENTRATION (PC/CU.M)

Z DIRECTION = 505.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.03	0.03
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.05	0.06	0.11	0.11
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.02	0.03	0.02	0.02	0.01	0.02	0.02
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.00
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 442.1 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.07	0.08	0.12	0.13
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.02	0.02	0.04	0.04	0.02	0.01	0.02	0.02
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.01	0.01	0.00	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 439.7 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.11	0.17	0.18
Y=-284.1 M	0.0	0.0	0.0	0.0	0.01	0.01	0.03	0.02	0.0	0.0	0.0	0.13	0.45	0.62	0.66
Y= 0.0 M	0.0	0.0	0.0	0.0	0.08	0.07	0.11	0.13	0.13	0.14	0.12	0.07	0.07	0.11	0.12
Y= 284.1 M	0.0	0.0	0.0	0.0	0.01	0.01	0.03	0.03	0.03	0.05	0.04	0.01	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 355.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.43	0.73	0.93	1.02	1.05
Y=-284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.27	0.25	0.87	2.54	3.66	3.53	3.65	3.76	3.74
Y= 0.0 M	0.0	0.0	0.0	0.0	0.31	0.86	1.16	1.21	1.24	1.33	1.12	0.72	0.61	0.66	0.68
Y= 284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.27	0.25	0.30	0.31	0.19	0.06	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.02	0.03	0.02	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 252.5 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.26	0.55	1.55	1.58	1.67	1.59	1.59
Y=-284.1 M	0.0	0.01	0.18	0.57	0.94	1.21	1.36	22.66	21.52	17.80	13.48	10.11	8.17	7.30	7.11
Y= 0.0 M	0.0	1.08	3.90	5.72	6.10	6.03	5.52	5.86	5.64	5.59	3.86	1.95	1.30	1.26	1.23
Y= 284.1 M	0.0	0.01	0.18	0.57	0.94	1.21	1.36	1.25	1.34	1.16	0.64	0.14	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04	0.14	0.13	0.06	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 150.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.14	0.44	0.74	0.93	1.03	1.05
Y=-284.1 M	0.0	0.31	1.16	1.82	2.10	2.26	2.34	2.34	2.87	4.29	4.64	4.17	3.86	3.76	3.73
Y= 0.0 M	35.45	32.69	25.20	18.21	13.57	11.18	10.12	9.82	9.44	7.58	4.45	1.47	0.61	0.59	0.54
Y= 284.1 M	0.0	0.31	1.16	1.82	2.10	2.26	2.34	2.34	2.30	2.07	1.13	0.28	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.03	0.05	0.03	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 65.3 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04	0.19	0.20	0.22
Y=-284.1 M	0.0	0.02	0.27	0.77	1.21	1.57	1.72	1.72	1.45	0.91	0.34	0.34	0.53	0.71	0.73
Y= 0.0 M	0.0	1.01	5.85	7.61	7.67	7.53	7.21	7.03	6.68	5.29	2.59	0.54	0.06	0.07	0.05
Y= 284.1 M	0.0	0.02	0.27	0.77	1.21	1.57	1.72	1.72	1.67	1.47	0.76	0.16	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.01	0.01	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 12.9 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.03	0.06	0.07
Y=-284.1 M	0.0	0.0	0.0	0.17	0.65	1.12	1.22	1.20	1.25	1.13	0.42	0.09	0.11	0.19	0.21
Y= 0.0 M	0.0	0.0	0.0	1.60	3.74	4.90	4.78	4.55	4.18	2.95	1.08	0.12	0.02	0.04	0.02
Y= 284.1 M	0.0	0.0	0.0	0.17	0.65	1.12	1.22	1.20	1.11	0.84	0.33	0.04	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.01	0.00	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 0.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.05	0.06
Y=-284.1 M	0.0	0.0	0.0	0.15	0.63	1.10	1.20	1.17	0.68	0.87	0.35	0.05	0.08	0.16	0.18
Y= 0.0 M	0.0	0.0	0.0	1.46	3.59	4.78	4.64	4.44	4.02	2.77	0.96	0.09	0.02	0.04	0.02
Y= 284.1 M	0.0	0.0	0.0	0.15	0.63	1.10	1.20	1.17	1.08	0.79	0.30	0.03	0.0	0.0	0.0
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.01	0.00	0.0	0.0	0.0
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

CHECK/SEC= 4999.76 5074.32 5136.58 5039.74 4868.68 4858.25 4826.15 7373.73 7645.72 7104.28 5335.32 3623.04 3029.45 2950.56 2920.62

Table 6.9 Continuation

(Θ = 80 min)

(Ω = 90 min)

X DIRECTION (METERS)

0.0 337.7 1694.0 3006.9 6193.1 8306.0 9662.3 10000.0 10270.1 11355.2 13045.5 14554.5 16644.8 17725.9 18000.0

CONCENTRATION (MG/CU.M)

Z DIRECTION = 905.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.04
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.02	0.11	0.16	0.18
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.01	0.03	0.06	0.10	0.15	0.19	0.20
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.01	0.01	0.03	0.05	0.06	0.07
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.01	0.01
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 492.1 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.04	0.04
Y=-284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.0	0.0	0.0	0.10	0.13	0.15	0.21
Y= 0.0 M	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.02	0.04	0.07	0.11	0.17	0.21	0.22
Y= 284.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.00	0.01	0.01	0.03	0.05	0.07	0.07
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.01	0.01
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 439.7 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.12	0.15	0.20
Y=-284.1 M	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.03	0.0	0.0	0.0	0.24	0.41	0.81	0.86
Y= 0.0 M	0.0	0.0	0.0	0.0	0.08	0.07	0.11	0.12	0.15	0.16	0.24	0.28	0.51	0.60	0.62
Y= 284.1 M	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.03	0.03	0.05	0.08	0.12	0.15	0.16	0.17
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	0.03	0.03
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 355.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.13	0.43	0.75	0.97	1.08	1.11
Y=-284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.26	0.28	0.87	2.53	3.87	4.40	4.55	4.47	4.46
Y= 0.0 M	0.0	0.0	0.0	0.0	0.32	0.86	1.12	1.18	1.23	1.45	1.82	2.17	2.29	2.45	2.52
Y= 284.1 M	0.0	0.0	0.0	0.0	0.05	0.17	0.26	0.28	0.29	0.34	0.40	0.46	0.52	0.56	0.57
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.02	0.05	0.09	0.11	0.12	0.12
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 252.5 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.04
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.26	0.55	1.00	1.53	2.08	2.13	2.14
Y=-284.1 M	0.0	0.01	0.10	0.57	0.95	1.21	1.33	22.63	21.52	17.64	14.18	11.48	9.85	9.03	8.85
Y= 0.0 M	0.0	1.08	3.91	5.70	6.14	6.00	5.81	5.76	5.65	6.05	6.18	6.10	5.93	5.79	5.75
Y= 284.1 M	0.0	0.01	0.10	0.57	0.95	1.21	1.33	1.36	1.22	1.25	1.30	1.37	1.42	1.45	1.46
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04	0.14	0.20	0.23	0.25	0.26	0.26
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 150.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.05	0.05
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.14	0.47	0.83	1.05	1.23	1.24
Y=-284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.29	2.25	2.88	4.53	5.75	6.22	6.25	6.15	6.16
Y= 0.0 M	35.45	32.88	25.22	18.18	13.63	11.12	9.64	9.09	9.50	8.87	8.16	7.59	7.16	6.92	6.86
Y= 284.1 M	0.0	0.31	1.16	1.81	2.12	2.24	2.29	2.29	2.30	2.31	2.29	2.26	2.26	2.26	2.25
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.03	0.09	0.17	0.23	0.26	0.27
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 65.3 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.05	0.06
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.16	0.32	0.42	0.45
Y=-284.1 M	0.0	0.02	0.27	0.76	1.22	1.55	1.72	1.76	1.57	1.36	1.76	2.36	2.85	3.07	3.11
Y= 0.0 M	0.0	1.80	5.86	7.59	7.72	7.44	7.23	7.17	7.12	6.92	6.63	6.37	6.17	6.03	5.98
Y= 284.1 M	0.0	0.02	0.27	0.76	1.22	1.55	1.72	1.76	1.79	1.92	2.08	2.21	2.29	2.32	2.32
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.05	0.12	0.19	0.23	0.24
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 12.9 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.05	0.05
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.10	0.16	0.25	0.31	0.32
Y=-284.1 M	0.0	0.0	0.0	0.17	0.65	1.10	1.35	1.41	1.40	1.93	2.00	2.13	2.33	2.43	2.45
Y= 0.0 M	0.0	0.0	0.0	1.62	3.74	4.84	5.24	5.31	5.36	5.53	5.63	5.64	5.58	5.41	5.34
Y= 284.1 M	0.0	0.0	0.0	0.17	0.65	1.10	1.35	1.41	1.46	1.63	1.86	2.08	2.22	2.23	2.27
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.03	0.08	0.15	0.22	0.25	0.26
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Z DIRECTION = 0.0 M

Y=-664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.05	0.05
Y=-519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.10	0.18	0.24	0.30	0.32
Y=-284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	1.05	1.70	1.94	2.09	2.30	2.39	2.41
Y= 0.0 M	0.0	0.0	0.0	1.48	3.58	4.72	5.14	5.22	5.27	5.45	5.57	5.59	5.54	5.37	5.30
Y= 284.1 M	0.0	0.0	0.0	0.15	0.63	1.08	1.34	1.40	1.45	1.63	1.86	2.07	2.21	2.23	2.21
Y= 519.1 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.03	0.08	0.15	0.22	0.25	0.26
Y= 664.4 M	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

ENERGY/SEC = 4999.76 5070.20 5144.46 5025.23 4899.54 4824.38 4777.76 7769.83 7774.45 7793.37 7755.09 7704.23 7642.32 7577.87 7550.79

Sensivity Analysis

The merit of any model depends on its ability to represent the actual physics and chemistry.

It is evident from the diffusion equation that both the turbulent diffusivities and the velocity profiles have a direct influence on the values calculated by the present model. This is the reason why, as was previously discussed, general expressions are provided for the turbulent diffusivities and the velocity profiles by means of several parameters. In this way, different functional relationships can be easily tested with the present model.

All the parameters given in Table 6.10 must be supplied as input information by the user. Therefore, these parameters can be selected to obtain the best set which will represent the actual conditions of the problem to solve.

The influence of these parameters on the concentration distribution is discussed next. The basis of this analysis is the parametric study on hypothetical cases previously presented.

The influence of AM can be observed from a comparison between cases 2 and 3. As the wind velocity increases, i.e., AM decreases, the values for the mean concentration at a same position decrease. This effect is more evident for the concentration distribution at the ground level.

Table 6.10 : Parameters in Turbulent Diffusivity and Velocity Profiles

ISTB	the stability class
ALPHA	the coefficient in the equation for the y-component of the turbulent diffusivity vector
UST	the geostrophic wind speed
AM	the exponent in the power law equation for the velocity profiles
P	the constant that determines the direction of the mean wind velocity
TCH	the parameter that specifies the time required for the y-component of the wind velocity to change from its value at t=0 to its maximum value, P•u

A comparison between cases 1 and 3 shows the effect of alpha on the concentration distribution. An increase in alpha (Case 3) means an increase in the y-component of the turbulent diffusivity vector, and thus more dispersion occurs in the y-direction. The net effect, as can be observed in Tables 6.4 and 6.5, is that the

concentration at the centerline decreases, and at any y different than zero increases, when compared to the values at same x and z for case 1.

The effect of the chemical reaction on the concentration distribution can be observed from a comparison between cases 3 and 4. The concentration values at any location, x, y, z, in case 4, where a chemical reaction occurs, are smaller than the values in case 3, where the rate of reaction is zero.

A comparison between cases 4, 5, and 6 shows the effect of the atmospheric stability on the concentration distribution. As the atmospheric stability increases, the concentration values at the centerline increase, and the concentration distribution at ground level decreases. It can also be observed that as the instability increases, the pollutant dispersion increases, and the x-position of the maximum ground level concentration moves closer to the source.

Case 7 shows the effect of the stack height on the concentration distribution. It is evident that as the stack height increases, the concentration values at ground level decrease (compare with case 4).

Finally, the effect of the y-component of the wind velocity (case 8) is shown in Tables 6.6 and 6.7. In this case, V was directed in the positive y-direction (from

-YMAX to YMAX), and the net effect is to move the plume more towards that direction.

From this analysis it can be concluded that the present model responds to variations in atmospheric conditions. Furthermore, the results indicate good agreement when compared to an actual response one would expect.

There are two additional parameters that will also influence the results of the present work. Although they do not affect the solution as much as the previous ones, some attention should be devoted to them.

One arises because of the use of RKGS subroutine for solving the system of first-order ordinary differential equations. This parameter is the upper error bound, which must be supplied as input information by the user, and is called PRMT(4) in the computer program.

Neither the truncation errors nor estimates of them are obtained in the calculational procedure performed by "RKGS". Therefore, control of accuracy and adjustment of the step size is done by comparison of the results due to double and single step size calculations.

The procedure is the following: a test value δ (see RKGS [14]), which is an approximate measure for the local truncation error, is compared to the given tolerance PRMT(4). If δ is greater the PRMT(4), the step size or increment of integration of the independent variable is

halved, and the procedure starts again. However, if δ is less than PRMT(4), the results are assumed to be correct.

It can be observed that the larger the value of PRMT(4), the faster the integration is performed. This indicates a decrease in the computing time required, but there is a possibility of obtaining less accurate results.

In order to avoid this inaccuracy on the results, the value of PRMT(4) is usually given small, i.e., in the range of 10^{-3} to 10^{-5}. However, its value and the value for PRMT(3), the initial step size, are actually dependent on the problem to be solved. Unfortunately, there is no general formula to evaluate these parameters. Therefore, for each particular problem, their values have to be studied in order to obtain a fast and accurate solution.

In the present work, this study was performed in the following way: initially, a small value for PRMT(4) was given, i.e., 10^{-5}. Then, this upper error bound was increased and the results for the concentration distribution compared to the previous ones. This procedure was stopped when a change in the second decimal on the concentration values was observed. The corresponding PRMT(4) was then used thereafter, for all the other cases solved.

A similar procedure was performed to obtain the best value for PRMT(3). In this case, several values were

tested and the corresponding computing times compared. It should be pointed out that this parameter affects only the number of bisections done on it, which is also related to the given tolerance PRMT(4).

For the present study, the best values obtained for these two parameters are given in Table 6.11.

Table 6.11 : PRMT(3) and PRMT(4) Values Used in the Simulations

	Prairie Grass Runs	Hypothetical Cases
PRMT(3)	.05 min	2.5 min
PRMT(4)	.01 min	1.0 min

It can be observed that the values of PRMT(3) and PRMT(4) for the Prairie Grass runs are much smaller than those for the hypothetical cases. The reason being the much smaller dimensions in the three coordinate directions, and thus a smaller step size of integration and smaller upper error bound were needed.

Orthogonal collocation introduces a second parameter that can affect the solution of the model. It is evident that the number of equations increases as the number of

orthogonal points used to obtain the solution is increased. This situation will therefore increase the computer time requirements.

Having this in mind, the present method was developed for a variable number of orthogonal points in the x, y, and z directions. They must be supplied as input information by the user, and can be changed from one simulation to another. However, in the present program there is a restriction to use not more than 15 points in each direction and the product $(N_x+1)*N_y*N_z$ be less than 700. The reason being dimension and common statements presently used in the computer program. Actually, no limit exists except for computer capacities and time requirements to solve the problem.

A similar analysis to the one performed for PRMT(4) was done for the number of orthogonal points needed to obtain accurate results. It was concluded that 5 to 10 points in each direction were enough.

Facilities at U. of H. and Time Requirements

The computer facilities at the University of Houston consist of a UNIVAC 1108 digital computer at the University Computing Center and of an IBM 360 Model 44 digital computer in the Engineering Systems Simulation Laboratory of the Cullen College of Engineering.

The computer time required to simulate atmospheric diffusion by the present method depends on the type of problem to be solved. For all the hypothetical cases simulated, with the exception of cases 5 and 10, the ratio of CPU time to real time was about 1/93 on the UNIVAC and 1/16 on the IBM. Case 5 was solved with a ratio of 1/53 on the UNIVAC and 1/10 on the IBM, and the two sources case had a ratio of 1/46 and 1/7, respectively.

The computer time required to solve each of the Prairie Grass runs was higher than the hypothetical cases. The reason being the small dimensions in the x, y, z directions, and thus a very small diffusion time. This required, as it was previously discussed, a very small step size in the integration of the differential equations and a very small upper error bound. In these cases, the ratio of CPU time to real time was about 1/2 on the UNIVAC and 3/1 on the IBM..

Chapter VII

SUMMARY OF RESULTS AND RECOMMENDATIONS

Turbulent diffusion from single or multiple point sources in the atmosphere was successfully simulated using the K-theory and a new numerical technique, orthogonal collocation.

Excellent agreement was observed between simulated and experimental concentration profiles for ground level emission sources. The present model had also an excellent response to variations in atmospheric conditions. This was obtained by simulating hypothetical elevated source cases.

Empirical equations were used to describe the mean wind velocities and the turbulent diffusivities. Several parameters were included in these equations so that many atmospheric conditions can be simulated by the present technique.

The present method has several very significant advantages over other available methods, i.e.,

1.) A general 3-dimensional, unsteady state problem can be solved using a simpler numerical technique. Accurate results can be obtained in very reasonable amount of computer time.

2.) The method can handle multiple sources put at any position, depending only on the orthogonal points considered.

3.) Several meteorological effects are taken into consideration.

4.) Mean velocities and turbulent diffusivities can be functions of all three position coordinates, time, and meteorological conditions.

5.) Cases with or without an inversion layer, and with or without generation or deposition at the ground level can be solved.

6.) The concentration at the source or the emission rate can be given as input information. The method will also calculate the flux across y-z planes at x=constant.

7.) Chemical reactions in the atmosphere can be incorporated.

8.) Most of the assumptions involved in the present method are in the input information.

Although the present model gives an improved method for solving atmospheric diffusion problems, it should be extended such that any general case could be solved. These extensions should include:

1.) A better representation of true dispersion processes by means of improving the expressions for turbulent diffusivity and mean wind velocity profiles;

2.) The incorporation of more realistic chemical reactions and in general any type of removal processes;

3.) The incorporation of other atmospheric effects such as the Coriolis effect;

4.) Improvements in orthogonal collocation such as removing the restriction on the position of each point source; and

5.) Extension to area and line sources.

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APPENDIX

APPENDIX A

COMPUTER PROGRAM LISTING

The computer program used in the present work is shown next. All statements are written in Fortran IV. This program can be executed in IBM 360 or UNIVAC 1108 digital computers.

```
      C  ***************************************************************** MAIN  10
      C                                                                    MAIN  20
      C  MODEL FOR ATMOSPHERIC DIFFUSION BY ORTHOGONAL COLLOCATION         MAIN  30
      C                                                                    MAIN  40
      C  MIGUEL T. FLEISCHER                                               MAIN  50
      C                                                                    MAIN  60
      C  ***************************************************************** MAIN  70
      C                                                                    MAIN  80
      C                                                                    MAIN  90
      C  NOMENCLATURE                                                      MAIN 100
      C                                                                    MAIN 110
      C                                                                    MAIN 120
      C     TINIT,ENDS - INITIAL AND FINAL SIMULATION TIMES                MAIN 130
      C     Y          - CONCENTRATION (USED FOR RKGS)                     MAIN 140
      C     CC(I,J,K,L)- CONCENTRATION AT POINT (J,K,L) DUE PRIMARILY TO   MAIN 150
      C                  ITH. SOURCE (USED FOR OUTPUT)                     MAIN 160
      C     C(J,K,L)   - CONCENTRATION AT POINT (J,K,L)(USED FOR ZERO AND AVG)MAIN 170
      C     NX         - NUMBER OF POINTS IN X DIRECTION                   MAIN 180
      C     NY         - NUMBER OF POINTS IN Y DIRECTION                   MAIN 190
      C     NZ         - NUMBER OF POINTS IN Z DIRECTION                   MAIN 200
      C     XMAX(I)    - MAXIMUM DISTANCE FROM THE ITH. SOURCE IN THE X    MAIN 210
      C                  DIRECTION                                         MAIN 220
      C     YMAX       - MAXIMUM DISTANCE IN Y DIRECTION                   MAIN 230
      C     H          - MAXIMUM HEIGHT ABOVE TERRAIN                      MAIN 240
      C     AKY,AKZ    - TURBULENT EDDY DIFFUSIVITIES IN Y AND Z DIRECTIONS MAIN 250
      C     ALPHA      - CONSTANT USED TO CALCULATE AKY                    MAIN 260
      C     U,V,W      - COMPONENTS OF MEAN WIND VELOCITY VECTOR           MAIN 270
      C     UST,XM     - PARAMETERS IN U EXPRESSION                        MAIN 280
      C     TCH        - TIME WHEN V BECOMES 100 %                         MAIN 290
      C     P          - CONSTANT USED TO SPECIFY THE VALUE OF V           MAIN 300
      C     UGR        - VELOCITY AT GROUND LEVEL                          MAIN 310
      C     AK         - RATE OF REACTION                                  MAIN 320
      C     ISTB       - STABILITY CLASS (1 VERY UNSTABLE, 6 VERY STABLE)  MAIN 330
      C     INVRS      - 1 OR 0, IF 1 THERE IS INVERSION AT Z=H; IF 0 THERE ISMAIN 340
      C                  NO INVERSION                                      MAIN 350
```

```
C      NSRCS       - NUMBER OF SOURCES                                          MAIN 350
C      KS(I),LS(I)- POSITION OF ITH. SOURCE IN THE Y AND Z DIRECTIONS           MAIN 370
C      CO(I)       - CONCENTRATION AT ITH. SOURCE                               MAIN 380
C                                                                               MAIN 390
C                                                                               MAIN 400
       EXTERNAL FCT,OUTP                                                        MAIN 410
       DIMENSION PRMT(5),Y1(700),Y2(700),Y3(700),DERY1(700),DERY2(700),         MAIN 420
      1DERY3(700),AUX(8,700),EA(15),EB(15),EC(15),ROOT(15),VEC(15),             MAIN 430
      2X7(15),AKY(15),AKZ(15),DAK7(15),COEFK(4),DKN(4),TDFKN(4)                 MAIN 440
       DEFINE FILE 2(2000,225,U,IIPNT)                                          MAIN 450
       DEFINE FILE 3(200,225,U,IPOIN)                                           MAIN 460
       DEFINE FILE 4(200,225,U,IPOINT)                                          MAIN 470
       COMMON /BLK1/ A1(15,15),A2(15,15),A3(15,15),B1(15,15),B2(15,15),         MAIN 480
      1B3(15,15),R1(15),R3(15),R5(15),R6(15),R361(15),R362(15),APA1(15),        MAIN 490
      2A36I(15,15),Q(700),U(15),V(15),XXX(3,15),XYY(15),XZ7(15),XMAX(3),        MAIN 500
      3YMAX,H,AK,TCH,P,KS(3),LS(3),CO(3),NX,NY,N7,N1,N2,N3,KX,KY,K7,            MAIN 510
      4W1(15),W2(15),W3(15),NSRCS,IFLG,MFLG,CC(3,15,15,15),PRDEL,PRMT3,         MAIN 520
      5INVRS                                                                    MAIN 530
C                                                                               MAIN 540
C                                                                               MAIN 550
C  READ AND WRITE INPUT DATA                                                    MAIN 560
C                                                                               MAIN 570
C                                                                               MAIN 580
       DATA COEFK/2940.,540.,258.,90./                                          MAIN 590
       DATA DKN/125.,125.,100.,75./                                             MAIN 600
       WRITE(6,205)                                                             MAIN 610
       WRITE(6,206)                                                             MAIN 620
       READ(5,100) TINIT,ENDS,PRMT(3),PRMT(4)                                   MAIN 630
       WRITE(6,200) TINIT,ENDS,PRMT(3),PRMT(4)                                  MAIN 640
       READ(5,109) NSRCS                                                        MAIN 650
       WRITE(6,209) NSRCS                                                       MAIN 660
       READ(5,106) PRDEL                                                        MAIN 670
       WRITE(6,208) PRDEL                                                       MAIN 680
       READ(5,101) NX,NY,NZ                                                     MAIN 690
       WRITE(6,201) NX,NY,NZ                                                    MAIN 700
       READ(5,102) YMAX,H                                                       MAIN 710
```

```
      WRITE(6,202) YMAX,H                                               MAIN 720
      DO 85 I=1,NSRCS                                                   MAIN 730
      READ(5,104) KS(I),LS(I),CO(I),XMAX(I)                             MAIN 740
   85 WRITE(6,204) KS(I),LS(I),CO(I),XMAX(I)                            MAIN 750
      READ(5,105) ISTB,INVRS,ALPHA,AK                                   MAIN 760
      WRITE(6,207) ISTB,INVRS,ALPHA,AK                                  MAIN 770
      READ(5,103) UST,UGR,AM,TCH,P                                      MAIN 780
      WRITE(6,203) UST,UGR,AM,TCH,P                                     MAIN 790
C                                                                       MAIN 800
C                                                                       MAIN 810
C  INITIAL CONDITIONS                                                   MAIN 820
C                                                                       MAIN 830
C                                                                       MAIN 840
      NDIM=(NX+1)*NY*NZ                                                 MAIN 850
      PRMT3=PRMT(3)                                                     MAIN 860
      DO 51 I=1,NDIM                                                    MAIN 870
      Q(I)=0.                                                           MAIN 880
      Y1(I)=0.                                                          MAIN 890
      Y2(I)=0.                                                          MAIN 900
   51 Y3(I)=0.                                                          MAIN 910
      SUM=0.                                                            MAIN 920
      KK=NDIM-1                                                         MAIN 930
      DO 52 I=1,KK                                                      MAIN 940
      DERY1(I)=1./FLOAT(NDIM)                                           MAIN 950
   52 SUM=SUM+DERY1(I)                                                  MAIN 960
      DERY1(NDIM)=1.-SUM                                                MAIN 970
      DO 86 I=1,NDIM                                                    MAIN 980
      DERY2(I)=DERY1(I)                                                 MAIN 990
   86 DERY3(I)=DERY1(I)                                                 MAIN1000
      N1=NX+2                                                           MAIN1010
      N2=NY+2                                                           MAIN1020
      N3=NZ+2                                                           MAIN1030
      KX=NX+1                                                           MAIN1040
      KY=NY+1                                                           MAIN1050
      KZ=NZ+1                                                           MAIN1060
      DO 53 I=1,NSRCS                                                   MAIN1070
```

```
      DO 55 J=1,N1                                                      MAIN1090
      DO 53 K=2,KY                                                      MAIN1100
      DO 53 L=1,N3                                                      MAIN1110
   53 CC(I,J,K,L)=0.                                                    MAIN1120
C                                                                       MAIN1130
C                                                                       MAIN1140
C  CALCULATION OF ORTHOGONAL POINTS, QUADRATURE WEIGHTS, AND            MAIN1150
C  MATRICES A AND B                                                     MAIN1160
C                                                                       MAIN1170
C                                                                       MAIN1180
C  X DIRECTION                                                          MAIN1190
C                                                                       MAIN1200
C                                                                       MAIN1210
      CALL JCPI(NX,1,1,0.,0.,FA,FB,FC,ROOT)                             MAIN1220
      DO 20 I=1,N1                                                      MAIN1230
      XXX(1,I)=ROOT(I)*XMAX(1)                                          MAIN1240
      IF(NSRCS.EQ.1) GO TO 20                                           MAIN1250
      XXX(2,I)=ROOT(I)*XMAX(2)+XMAX(1)                                  MAIN1260
      IF(NSRCS.EQ.2) GO TO 20                                           MAIN1270
      XXX(3,I)=ROOT(I)*XMAX(3)+XMAX(2)                                  MAIN1280
   20 CONTINUE                                                          MAIN1290
      DO 60 I=1,N1                                                      MAIN1300
      CALL DEOPR(NX,1,1,I,1,FA,FB,FC,ROOT,VEC)                          MAIN1310
      DO 70 K=1,N1                                                      MAIN1320
   70 A1(I,K)=VEC(K)                                                    MAIN1330
      CALL DEOPR(NX,1,1,I,2,FA,FB,FC,ROOT,VEC)                          MAIN1340
      DO 80 K=1,N1                                                      MAIN1350
   80 B1(I,K)=VEC(K)                                                    MAIN1360
   60 CONTINUE                                                          MAIN1370
      CALL DEOPR(NX,1,1,I,3,FA,FB,FC,ROOT,W1)                           MAIN1380
C                                                                       MAIN1390
C                                                                       MAIN1400
C  Y DIRECTION                                                          MAIN1410
C                                                                       MAIN1420
C                                                                       MAIN1430
      CALL JCPI(NY,1,1,0.,0.,FA,FB,FC,ROOT)                             MAIN1440
```

```
144:          DO 21 I=1,N2                                                  MAIN1440
145:       21 XYY(I)=ROOT(I)*2.*YMAX-YMAX                                   MAIN1450
146:          DO 61 I=1,N2                                                  MAIN1460
147:          CALL DFOPR(NY,1,1,I,1,FA,FB,FC,ROOT,VEC)                      MAIN1470
148:          DO 71 K=1,N2                                                  MAIN1480
149:       71 A2(I,K)=VEC(K)                                                MAIN1490
150:          CALL DFOPR(NY,1,1,I,2,FA,FB,FC,ROOT,VEC)                      MAIN1500
151:          DO 81 K=1,N2                                                  MAIN1510
152:       81 B2(I,K)=VEC(K)                                                MAIN1520
153:       61 CONTINUE                                                      MAIN1530
154:          CALL DFOPR(NY,1,1,I,3,FA,FB,FC,ROOT,W2)                       MAIN1540
155:    C                                                                   MAIN1550
156:    C                                                                   MAIN1560
157:    C  Z DIRECTION                                                      MAIN1570
158:    C                                                                   MAIN1580
159:    C                                                                   MAIN1590
160:          CALL JCBI(NZ,1,1,0.,0.,FA,FB,FC,ROOT)                         MAIN1600
161:          DO 92 I=1,N3                                                  MAIN1610
162:       92 XZ(I)=ROOT(I)                                                 MAIN1620
163:          DO 22 I=1,N3                                                  MAIN1630
164:       22 XZZ(I)=ROOT(I)*H                                              MAIN1640
165:          DO 62 I=1,N3                                                  MAIN1650
166:          CALL DFOPR(NZ,1,1,I,1,FA,FB,FC,ROOT,VEC)                      MAIN1660
167:          DO 72 K=1,N3                                                  MAIN1670
168:       72 A3(I,K)=VEC(K)                                                MAIN1680
169:          CALL DFOPR(NZ,1,1,I,2,FA,FB,FC,ROOT,VEC)                      MAIN1690
170:          DO 82 K=1,N3                                                  MAIN1700
171:       82 B3(I,K)=VEC(K)                                                MAIN1710
172:       62 CONTINUE                                                      MAIN1720
173:          CALL DFOPR(NZ,1,1,I,3,FA,FB,FC,ROOT,W3)                       MAIN1730
174:    C                                                                   MAIN1740
175:    C                                                                   MAIN1750
176:    C  CALCULATION OF EXPRESSIONS USED IN MODEL                         MAIN1760
177:    C                                                                   MAIN1770
178:    C                                                                   MAIN1780
179:          IF(ISTD.GE.5) GO TO 10                                        MAIN1790
```

```
      U(1)=UGR                                                          MAIN1800
      TDEKN(ISTB)=DKN(ISTB)/H                                           MAIN1810
      TDSKN=1.-100./H                                                   MAIN1820
      DO 2 L=2,N3                                                       MAIN1830
      IF(XZ(L)-TDEKN(ISTB)) 11,12,12                                    MAIN1840
   11 AKZ(L)=COEFK(ISTB)*XZ(L)/TDEKN(ISTB)+60.                          MAIN1850
      DAKZ(L)=COEFK(ISTB)/DKN(ISTB)                                     MAIN1860
      U(L)=UST*(XZ(L)*H/DKN(ISTB))**AM                                  MAIN1870
      GO TO 16                                                          MAIN1880
   12 IF(XZ(L)-TDSKN) 13,13,14                                          MAIN1890
   13 AKZ(L)=COEFK(ISTB)+60.                                            MAIN1900
      DAKZ(L)=0.                                                        MAIN1910
      GO TO 15                                                          MAIN1920
   14 AKZ(L)=COEFK(ISTB)*H*(1.-XZ(L))/100.+60.                          MAIN1930
      DAKZ(L)=-COEFK(ISTB)/100.                                         MAIN1940
   15 U(L)=UST                                                          MAIN1950
   16 AKY(L)=ALPHA*(COEFK(ISTB)+60.)                                    MAIN1960
    2 CONTINUE                                                          MAIN1970
      GO TO 50                                                          MAIN1980
   10 IF(ISTB.EQ.6) GO TO 40                                            MAIN1990
      DO 3 L=2,N3                                                       MAIN2000
      AKZ(L)=60.                                                        MAIN2010
      U(L)=UST                                                          MAIN2020
      DAKZ(L)=0.                                                        MAIN2030
    3 AKY(L)=ALPHA*AKZ(L)                                               MAIN2040
      GO TO 50                                                          MAIN2050
   40 DO 4 L=2,N3                                                       MAIN2060
      AKZ(L)=30.                                                        MAIN2070
      U(L)=UST                                                          MAIN2080
      DAKZ(L)=0.                                                        MAIN2090
    4 AKY(L)=ALPHA*AKZ(L)                                               MAIN2100
   50 CONTINUE                                                          MAIN2110
      DO 41 L=2,KZ                                                      MAIN2120
      R3(L)=DAKZ(L)/H**2                                                MAIN2130
      R5(L)=AKY(L)/(4.*YMAX**2)                                         MAIN2140
   41 R6(L)=AKZ(L)/H**2                                                 MAIN2150
```

```
216:          DO 30 L=2,KZ                                                  MAIN2160
217:          R361(L)=R3(L)*A3(L,1)+R6(L)*P3(L,1)                           MAIN2170
218:       30 R362(L)=P3(L)*A3(L,N3)+R6(L)*R3(L,N3)                         MAIN2180
219:          DEN=A3(N3,1)*A3(1,N3)-A3(1,1)*A3(N3,N3)                       MAIN2190
220:          DO 31 I=2,KZ                                                  MAIN2200
221:       31 APA1(I)=(A3(1,1)*A3(N3,I)-A3(N3,1)*A3(1,I))/DEN               MAIN2210
222:          DO 32 L=2,KZ                                                  MAIN2220
223:          DO 32 I=2,KZ                                                  MAIN2230
224:       32 R36I(L,I)=R3(L)*A3(L,I)+R6(L)*P3(L,I)                         MAIN2240
225:   C                                                                    MAIN2250
226:   C                                                                    MAIN2260
227:   C  WRITE INITIAL CONDITIONS                                          MAIN2270
228:   C                                                                    MAIN2280
229:   C                                                                    MAIN2290
230:          MFLG=1                                                        MAIN2300
231:          IFLG=0                                                        MAIN2310
232:          PRMT(1)=0.                                                    MAIN2320
233:          PRMT(2)=0.                                                    MAIN2330
234:          CALL OUTP(0.,Y1,DERY1,0,NDIM,PRMT)                            MAIN2340
235:   C                                                                    MAIN2350
236:   C                                                                    MAIN2360
237:   C  INTEGRATION USING RKGS                                            MAIN2370
238:   C                                                                    MAIN2380
239:   C                                                                    MAIN2390
240:          MFLG=2                                                        MAIN2400
241:          PRMT(1)=TINIT                                                 MAIN2410
242:          PRMT(2)=ENDS                                                  MAIN2420
243:          IFLG=1                                                        MAIN2430
244:          CALL RKGS(PRMT,Y1,DERY1,NDIM,IHLF,FCT,OUTP,AUX)               MAIN2440
245:          IF(NSRGS.EQ.1) GO TO 59                                       MAIN2450
246:          IFLG=2                                                        MAIN2460
247:          CALL RKGS(PRMT,Y2,DERY2,NDIM,IHLF,FCT,OUTP,AUX)               MAIN2470
248:          IF(NSRGS.EQ.2) GO TO 59                                       MAIN2480
249:          IFLG=3                                                        MAIN2490
250:          CALL RKGS(PRMT,Y3,DERY3,NDIM,IHLF,FCT,OUTP,AUX)               MAIN2500
251:       59 CONTINUE                                                      MAIN2510
```

```
C                                                                       MAIN2520
  100 FORMAT(4F10.5)                                                    MAIN2530
  101 FORMAT(3I5)                                                       MAIN2540
  102 FORMAT(2F15.7)                                                    MAIN2550
  103 FORMAT(5F10.3)                                                    MAIN2560
  104 FORMAT(2I5,2F15.4)                                                MAIN2570
  105 FORMAT(2I2,F10.2,L12.3)                                           MAIN2580
  106 FORMAT(F10.4)                                                     MAIN2590
  109 FORMAT(I3)                                                        MAIN2600
  200 FORMAT(5X,'TINIT =',F5.1,5X,'ENDS =',F6.1,' MIN',5X,'PRMT(3) =',  MAIN2610
     1F6.2,' MIN',5X,'PRMT(4) = ',F8.5,/)                               MAIN2620
  201 FORMAT(5X,'NX =',I3,5X,'NY =',I3,5X,'NZ =',I3,/)                  MAIN2630
  202 FORMAT(5X,'YMAX =',F9.1,' M',5X,'H =',F8.2,' M',/)                MAIN2640
  203 FORMAT(5X,'UST =',F8.2,' M/MIN',5X,'UGR =',F8.2,' M/MIN',5X,'AM ='MAIN2650
     1,F7.3,5X,'TCH =',F5.1,' MIN',5X,'P =',F6.2)                       MAIN2660
  204 FORMAT(5X,'KS =',I3,3X,' LS =',I4,2X,'  CO =',F9.2,' MG/CU.M',3X, MAIN2670
     1'XMAX =',F9.1,' M',/)                                             MAIN2680
  205 FORMAT(10(/),35X,'INPUT DATA')                                    MAIN2690
  206 FORMAT(35X,'***** ****',//)                                       MAIN2700
  207 FORMAT(5X,'STABILITY CLASS =',I4,5X,' IWPS =',I3,5X,' ALPHA =',F7MAIN2710
     1.2,5X,' AK =',E10.2,' 1/MIN',/)                                   MAIN2720
  208 FORMAT(5X,'PRDEL =',F6.2,' MIN',/)                                MAIN2730
  209 FORMAT(5X,'NUMBER OF SOURCES =',I4,/)                             MAIN2740
      STOP                                                              MAIN2750
      END                                                               MAIN2760
```

```
      SUBROUTINE FCT(X,Y,DERY)                                          FCT   10
C                                                                       FCT   20
C                                                                       FCT   30
C  THIS SUBROUTINE COMPUTES THE DERIVATIVES(RIGHT HAND SIDES) OF THE    FCT   40
C  SYSTEM TO GIVEN VALUES OF X(TIME) AND Y(CONCENTRATION)               FCT   50
C                                                                       FCT   60
C                                                                       FCT   70
      DIMENSION Y(700),DERY(700),PAC(700),CZ0(700),CZ1(700),CZ2(700),   FCT   80
     1CZI(700),CYK(700),R2(15),R52I(15,15,15),CCC(15,15)                FCT   90
      COMMON /BLK1/ A1(15,15),A2(15,15),A3(15,15),B1(15,15),B2(15,15),  FCT  100
     1B3(15,15),R1(15),R3(15),R5(15),R6(15),R361(15),R362(15),APA1(15), FCT  110
     2R36I(15,15),U(700),U(15),V(15),XXX(3,15),XYY(15),XZZ(15),XMAX(3), FCT  120
     3YMAX,H,AK,TCH,P,KS(3),LS(3),CO(3),NX,NY,NZ,N1,N2,N3,KX,KY,KZ,      FCT  130
     4W1(15),W2(15),W3(15),NSRCS,IFLG,MFLG,CC(3,15,15,15),PRDEL,PRMT3,  FCT  140
     5INVRS                                                             FCT  150
      INTEGER VAR1,VAR2,VAR3,VAR4,VAR5,VAR6,VAR7                        FCT  160
      NDIM=(NX+1)*NY*NZ                                                 FCT  170
      DO 4 L=2,KZ                                                       FCT  180
    4 R1(L)=U(L)/XMAX(IFLG)                                             FCT  190
C                                                                       FCT  200
C  VARIATION IN THE V VELOCITY                                          FCT  210
C                                                                       FCT  220
      IF(X-TCH) 1,2,2                                                   FCT  230
    1 CONTINUE                                                          FCT  240
      DO 5 L=2,KZ                                                       FCT  250
      V(L)=P*U(L)*(X/TCH)                                               FCT  260
    5 R2(L)=V(L)/(2.*YMAX)                                              FCT  270
      GO TO 3                                                           FCT  280
    2 CONTINUE                                                          FCT  290
      DO 6 L=2,KZ                                                       FCT  300
      V(L)=P*U(L)                                                       FCT  310
    6 R2(L)=V(L)/(2.*YMAX)                                              FCT  320
    3 CONTINUE                                                          FCT  330
C                                                                       FCT  340
C  COMPUTATION OF THE DERIVATIVES                                       FCT  350
```

```
      C                                                                 FCT  360
            DO 33 L=2,KZ                                                FCT  370
            DO 33 K=2,KY                                                FCT  380
            DO 33 I=2,KY                                                FCT  390
         33 R52I(L,K,I)=R5(L)*R2(K,I)-R2(L)*A2(K,I)                     FCT  400
            DO 39 LL=1,NDIM                                             FCT  410
            CZ0(LL)=0.                                                  FCT  420
            CZI(LL)=0.                                                  FCT  430
            CZ2(LL)=0.                                                  FCT  440
         39 CYK(LL)=0.                                                  FCT  450
            J=1                                                         FCT  460
            JJ=KK                                                       FCT  470
            IF(IFLG.EQ.1) GO TO 35                                      FCT  480
            IX=IFIX(X/(PRMT3-.01))                                      FCT  490
            IIBK=(IFLG-2)*97+(IX+1)                                     FCT  500
            READ(4'IIBK) ((CCC(K,L),K=2,KY),L=1,N3)                     FCT  510
         35 CONTINUE                                                    FCT  520
            DO 51 LK=2,KY                                               FCT  530
            DO 51 LZ=2,KZ                                               FCT  540
            DO 50 LJ=J,JJ                                               FCT  550
            VAR1=KS(IFLG-1)                                             FCT  560
            VAR2=LS(IFLG-1)                                             FCT  570
            VAR3=LJ-(J-1)+1                                             FCT  580
            IF(IFLG.EQ.1) GO TO 40                                      FCT  590
            IF(LK.EQ.KS(IFLG).AND.LZ.EQ.LS(IFLG)) GO TO 10              FCT  600
            PAC(LJ)=0.                                                  FCT  610
            IF(CCC(VAR1,VAR2).GT.0.) PAC(LJ)=CCC(LK,LZ)*A1(VAR3,1)      FCT  620
            GO TO 20                                                    FCT  630
         10 PAC(LJ)=C0(IFLG)*A1(VAR3,1)                                 FCT  640
            IF(CCC(VAR1,VAR2).GT.0.) PAC(LJ)=PAC(LJ)+CCC(LK,LZ)*A1(VAR3,1)  FCT  650
            GO TO 20                                                    FCT  660
         40 IF(LK.EQ.KS(1).AND.LZ.EQ.LS(1)) GO TO 11                    FCT  670
            PAC(LJ)=0.                                                  FCT  680
            GO TO 20                                                    FCT  690
         11 PAC(LJ)=C0(1)*A1(VAR3,1)                                    FCT  700
         20 CONTINUE                                                    FCT  710
```

```
      DO 60 I=1,KX                                                                  FCT  720
      VAR4=I+1                                                                      FCT  730
      VAR5=I+J-1                                                                    FCT  740
   60 PAC(LJ)=PAC(LJ)+A1(VAR3,VAR4)*Y(VAR5)                                         FCT  750
      DO 70 I=2,KZ                                                                  FCT  760
      VAR6=LJ+KX*(I-LZ)                                                             FCT  770
      CZ2(LJ)=CZ2(LJ)+APA1(I)*Y(VAR6)*FLOAT(INVRS)                                  FCT  780
      CZ0(LJ)=CZ0(LJ)+A3(1,I)*Y(VAR6)                                              FCT  790
   70 CZI(LJ)=CZI(LJ)+R36I(LZ,I)*Y(VAR6)                                            FCT  800
      CZI(LJ)=(-A3(1,N3)*CZ2(LJ)-CZ0(LJ))/A3(1,1)                                   FCT  810
      DO 80 I=2,KY                                                                  FCT  820
      VAR7=LJ+(I-LK)*(KZ-1)*KX                                                      FCT  830
   80 CYK(LJ)=CYK(LJ)+R52I(LZ,LK,I)*Y(VAR7)                                         FCT  840
   50 DERY(LJ)=-R1(LZ)*PAC(LJ)+R361(LZ)*CZ1(LJ)+R362(LZ)*CZ2(LJ)+CZI(LJ)FCT  850
     1+CYK(LJ)+Q(LJ)-AK*Y(LJ)                                                       FCT  860
      J=JJ+1                                                                        FCT  870
      JJ=J+KX-1                                                                     FCT  880
   51 CONTINUE                                                                      FCT  890
      RETURN                                                                        FCT  900
      END                                                                           FCT  910
```

```
      SUBROUTINE JCBI(N,NO,N1,AL,BE,FA,FP,FC,ROOT)                      JCBI  10
C                                                                       JCBI  20
C                                                                       JCBI  30
C  THIS SUBROUTINE COMPUTES THE ROOTS OF AN NTH-DEGREE JACOBI POLYNOMIALJCBI  40
C  AND THE DERIVATIVES OF THE POLYNOMIAL AT THESE POINTS                JCBI  50
C                                                                       JCBI  60
C                                                                       JCBI  70
C     N           - THE NUMBER OF INTERIOR POINTS                       JCBI  80
C     NO          - 1 OR 0 IF X=0 IS INCLUDED OR NOT                    JCBI  90
C     N1          - SAME AS NO, FOR THE POINT X=1                       JCBI 100
C     AL,BE       - THE QUANTITIES ALFA AND BETA FOR THE WEIGHTING      JCBI 110
C                   FUNCTION                                            JCBI 120
C     FA,FB,FC    - THE FIRST,SECOND AND THIRD DERIVATIVES OF THE       JCBI 130
C                   POLYNOMIAL AT THE ROOTS                             JCBI 140
C     ROOT        - OUTPUT ARRAY CONTAINING THE N+NO+N1 ROOTS OF THE    JCBI 150
C                   POLYNOMIAL                                          JCBI 160
C                                                                       JCBI 170
C                                                                       JCBI 180
      DIMENSION FA(1),FB(1),FC(1),ROOT(1)                               JCBI 190
      AB=AL+BE                                                          JCBI 200
      AD=BE-AL                                                          JCBI 210
      AP=BE*AL                                                          JCBI 220
      FA(1)=(AD/(AB+2.)+1.)/2.                                          JCBI 230
      FB(1)=0.                                                          JCBI 240
      DO 10 I=2,N                                                       JCBI 250
      Z1=FLOAT(I)-1.                                                    JCBI 260
      Z=AB+2.*Z1                                                        JCBI 270
      FA(I)=(AB/Z*AD/(Z+2.)+1.)/2.                                      JCBI 280
      IF(I-2)  11,12,11                                                 JCBI 290
12    FB(I)=(AB+AP+Z1)/Z/Z/(Z+1.)                                       JCBI 300
      GOTO 10                                                           JCBI 310
11    Z=Z*Z                                                             JCBI 320
      Y=Z1*(AB+Z1)                                                      JCBI 330
      Y=Y*(AP+Y)                                                        JCBI 340
      FB(I)=Y/Z/(Z-1.)                                                  JCBI 350
```

```
36:   10    CONTINUE                                                    JCBI 360
37:         X=0.                                                        JCBI 370
38:         DO 20  I=1,N                                                JCBI 380
39:         I1=I-1                                                      JCBI 390
40:   25    XD=0.                                                       JCBI 400
41:         XN=1.                                                       JCBI 410
42:         XD1=0.                                                      JCBI 420
43:         XN1=0.                                                      JCBI 430
44:         DO 30  J=1,N                                                JCBI 440
45:         XP=(FA(J)-X)*XN-FB(J)*XD                                    JCBI 450
46:         XP1=(FA(J)-X)*XN1-FB(J)*XD1-XN                              JCBI 460
47:         XD=XN                                                       JCBI 470
48:         XD1=XN1                                                     JCBI 480
49:         XN=XP                                                       JCBI 490
50:   30    XN1=XP1                                                     JCBI 500
51:         ZC=1.                                                       JCBI 510
52:         Z=XN/XN1                                                    JCBI 520
53:         IF(I1) 21,21,22                                             JCBI 530
54:   22    DO23  J=1,I1                                                JCBI 540
55:   23    ZC=ZC-Z/(X-ROOT(J))                                         JCBI 550
56:   21    Z=Z/ZC                                                      JCBI 560
57:         X=X-Z                                                       JCBI 570
58:         IF( ABS(Z)-1.E-7 ) 26,26,25                                 JCBI 580
59:   26    ROOT(I)=X                                                   JCBI 590
60:         X=X+0.0005                                                  JCBI 600
61:   20    CONTINUE                                                    JCBI 610
62:         NT=N+N0+N1                                                  JCBI 620
63:         IF(N0-1)  35,36,35                                          JCBI 630
64:   36    DO 42 I=1,N                                                 JCBI 640
65:         J=N+1-I                                                     JCBI 650
66:   42    ROOT(J+1) =ROOT(J)                                          JCBI 660
67:         ROOT(1)=0.                                                  JCBI 670
68:   35    IF(N1-1) 38,37,38                                           JCBI 680
69:   37    ROOT(NT)=1.                                                 JCBI 690
70:   38    DO 40 I=1,NT                                                JCBI 700
71:         X=ROOT(I)                                                   JCBI 710
```

```
72:           FA(I)=1.                                                  JCBI 720
73:           FB(I)=0.                                                  JCBI 730
74:           FC(I)=0.                                                  JCBI 740
75:           DO 40 J=1,NT                                              JCBI 750
76:           IF(J-I) 41,40,41                                          JCBI 760
77:    41     Y=X-ROOT(J)                                               JCBI 770
78:           FC(I)=Y*FC(I)+3.*FB(I)                                    JCBI 780
79:           FB(I)=Y*FB(I)+2.*FA(I)                                    JCBI 790
80:           FA(I)=Y*FA(I)                                             JCBI 800
81:    40     CONTINUE                                                  JCBI 810
82:           RETURN                                                    JCBI 820
83:           END                                                       JCBI 830
```

```
      SUBROUTINE DEQPR( J,N0,N1,I,ID,FA,FB,FC,ROOT,VECT)                DEQP  10
C                                                                       DEQP  20
C                                                                       DEQP  30
C  THIS SUBROUTINE CALCULATES THE A AND B MATRICES AND THE QUADRATURE   DEQP  40
C  WEIGHTS FROM THE QUANTITIES DERIVED IN SUBROUTINE JCBI               DEQP  50
C                                                                       DEQP  60
C                                                                       DEQP  70
C     N,N0,N1     - SAME AS JCBI                                        DEQP  80
C     I           - DIFFERENTIAL OPERATOR AT X=ROOT(I)                  DEQP  90
C     ID          - INDICATOR, I.E. 1 FOR MATRIX A, 2 FOR MATRIX B,     DEQP 100
C                   3 FOR QUADRATURE WEIGHTS W                          DEQP 110
C     FA,FB,FC    - COMPUTED IN JCBI                                    DEQP 120
C     ROOT        - COMPUTED IN JCBI                                    DEQP 130
C     VECT        - CONTAINS THE COMPUTED VECTOR                        DEQP 140
C                                                                       DEQP 150
C                                                                       DEQP 160
      DIMENSION FA(1),FB(1),FC(1),ROOT(1),VECT(1)                       DEQP 170
      NT=N+N0+N1                                                        DEQP 180
      IF(ID-3) 1,10,10                                                  DEQP 190
1     DO 20 J=1,NT                                                      DEQP 200
      IF(J-I) 21,2,21                                                   DEQP 210
2     IF(ID-1) 5,4,5                                                    DEQP 220
4     VECT(I)=FB(I)/FA(I)/2.                                            DEQP 230
      GOTO 20                                                           DEQP 240
5     VECT(I)=FC(I)/FA(I)/3.                                            DEQP 250
      GOTO 20                                                           DEQP 260
21    Y=ROOT(I)-ROOT(J)                                                 DEQP 270
      VECT(J)=FA(I)/FA(J)/Y                                             DEQP 280
      IF(ID-2) 20,22,20                                                 DEQP 290
22    VECT(J)=VECT(J)*(FB(I)/FA(I)-2./Y)                                DEQP 300
20    CONTINUE                                                          DEQP 310
      GOTO 50                                                           DEQP 320
10    Y=0.                                                              DEQP 330
      IF(ID-4) 31,30,31                                                 DEQP 340
31    DO 25 J=1,NT                                                      DEQP 350
```

```
36:          X=ROOT(J)                                              DEOP 360
37:          AX=X*(1.-X)                                            DEOP 370
38:          IF(NO) 26,27,26                                        DEOP 380
39:    27    AX=AX/X/X                                              DEOP 390
40:    26    IF(N1) 28,29,23                                        DEOP 400
41:    29    AX=AX/(1.-X)/(1.-X)                                    DEOP 410
42:    28    VECT(J)=AX/FA(J)/FA(J)                                 DEOP 420
43:    25    Y=Y+VECT(J)                                            DEOP 430
44:          GOTO 50                                                DEOP 440
45:    30    DO 35 J=1,NT                                           DEOP 450
46:          X=ROOT(J)                                              DEOP 460
47:          IF(NO) 36,37,36                                        DEOP 470
48:    37    AX=1./X                                                DEOP 480
49:    36    IF(N1) 38,39,38                                        DEOP 490
50:    39    AX=1./(1.-X)                                           DEOP 500
51:    38    VECT(J)=AX/FA(J)/FA(J)                                 DEOP 510
52:    35    Y=Y+VECT(J)                                            DEOP 520
53:    60    DO 61  J=1,NT                                          DEOP 530
54:    61    VECT(J)=VECT(J)/Y                                      DEOP 540
55:    50    RETURN                                                 DEOP 550
56:          END                                                    DEOP 560
```

```
      SUBROUTINE OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                          OUTP  10
C                                                                       OUTP  20
C                                                                       OUTP  30
C  THIS SUBROUTINE GIVES THE OUTPUT OF THE MODEL                        OUTP  40
C                                                                       OUTP  50
C                                                                       OUTP  60
C     PRDEL       - THE INTERVAL AT WHICH THE RESULTS WILL BE PRINTED   OUTP  70
C     T OR THETA - TIME BETWEEN THE POLLUTANT RELEASE(TIMIT) AND THE    OUTP  80
C                  INITIATION OF THE AVERAGING TIME                     OUTP  90
C     OMEGA       - END OF THE AVERAGING TIME                           OUTP 100
C     CX(I,J)     - FLUX ACROSS Y-Z PLANE AT X' JTH. POINT DUE TO ITH.  OUTP 110
C                   AND PRECEDING SOURCES                               OUTP 120
C                                                                       OUTP 130
C                                                                       OUTP 140
      DIMENSION PRMT(5),Y(700),DERY(700),CZ0(700),CZ1(700),CZ2(700),    OUTP 150
     1C(15,15,15),CX(3,15),IHL(3,50)                                    OUTP 160
      COMMON /BLK1/ A1(15,15),A2(15,15),A3(15,15),B1(15,15),B2(15,15),  OUTP 170
     1B3(15,15),R1(15),R3(15),R5(15),R6(15),R361(15),R362(15),APA1(15), OUTP 180
     2R36I(15,15),J(700),U(15),V(15),XXX(3,15),XYY(15),XZZ(15),XMAX(3), OUTP 190
     3YMAX,H,AK,TCH,P,KS(3),LS(3),CO(3),NX,NY,NZ,N1,N2,N3,KX,KY,KZ,     OUTP 200
     4W1(15),W2(15),W3(15),NSRCS,IFLG,MFLG,CC(3,15,15,15),PRDEL,PRMT3,  OUTP 210
     5INVRC                                                             OUTP 220
      INTEGER VAR10,VAR11,VAR12,VAR13,VAR14,VAR15                       OUTP 230
      IFLAG=IFLG                                                        OUTP 240
      IF(MFLG.EQ.1) GO TO 15                                            OUTP 250
      IF(NSRCS.NE.1) GO TO 70                                           OUTP 260
      IF(X.EQ.0.0) IIII=0                                               OUTP 270
      IF(X.EQ.0.0) GO TO 71                                             OUTP 280
      AAI=FLOAT(IIII)                                                   OUTP 290
      AAI1=AAI-X/PRDEL                                                  OUTP 300
      IA1=IFIX(AAI1*100.)                                               OUTP 310
      IF(IA1.EQ.0) GO TO 71                                             OUTP 320
      GO TO 800                                                         OUTP 330
   70 IF(X.EQ.0.0) II=0                                                 OUTP 340
      IF(X.EQ.0.0) GO TO 71                                             OUTP 350
```

```
      AI=FLOAT(II)                                                      OUTP 360
      AI1=AI-X/PRMT(3)                                                  OUTP 370
      I1=IFIX(AI1*100.)                                                 OUTP 380
      IF(I1.EQ.0) GO TO 71                                              OUTP 390
      GO TO 800                                                         OUTP 400
   71 CONTINUE                                                          OUTP 410
      J=1                                                               OUTP 420
      JJ=KX                                                             OUTP 430
      DO 2 ID=1,NY                                                      OUTP 440
      DO 1 LJ=J,JJ                                                      OUTP 450
      CZ0(LJ)=0.                                                        OUTP 460
      CZ2(LJ)=0.                                                        OUTP 470
      DO 5 I=2,KZ                                                       OUTP 480
      VAR10=LJ+KX*(I-2)                                                 OUTP 490
      CZ2(LJ)=CZ2(LJ)+APA1(I)*Y(VAR10)*FLOAT(INVRS)                     OUTP 500
    5 CZ0(LJ)=CZ0(LJ)+A3(1,I)*Y(VAR10)                                  OUTP 510
      CZ1(LJ)=(-A3(1,N3)*CZ2(LJ)-CZ0(LJ))/A3(1,1)                       OUTP 520
    1 CONTINUE                                                          OUTP 530
      J=ID*NZ*KX+1                                                      OUTP 540
      JJ=J+KX-1                                                         OUTP 550
    2 CONTINUE                                                          OUTP 560
      IND=2                                                             OUTP 570
      M1=1                                                              OUTP 580
      M2=KX                                                             OUTP 590
      DO 10 K=2,KY                                                      OUTP 600
      J=2                                                               OUTP 610
      DO 21 I=M1,M2                                                     OUTP 620
      C(J,K,1)=CZ1(I)                                                   OUTP 630
   21 J=J+1                                                             OUTP 640
      M3=M1                                                             OUTP 650
      M4=M2                                                             OUTP 660
      DO 20 L=2,KZ                                                      OUTP 670
      J=2                                                               OUTP 680
      DO 31 I=M3,M4                                                     OUTP 690
      C(J,K,L)=Y(I)                                                     OUTP 700
   31 J=J+1                                                             OUTP 710
```

```
 72:          M3=M4+1                                                    OUTP 720
 73:          M4=IND*KX                                                  OUTP 730
 74:          IND=IND+1                                                  OUTP 740
 75:       20 CONTINUE                                                   OUTP 750
 76:          J=2                                                        OUTP 760
 77:          DO 22 I=M1,M2                                              OUTP 770
 78:          C(J,K,N3)=CZ2(I)                                           OUTP 780
 79:       22 J=J+1                                                      OUTP 790
 80:          M1=M3                                                      OUTP 800
 81:          M2=M4                                                      OUTP 810
 82:       10 CONTINUE                                                   OUTP 820
 83:          CALL ZERO(C)                                               OUTP 830
 84:          IF(NSRCS.EQ.1) GO TO 65                                    OUTP 840
 85:          IX=IFIX(X/(PRMT3-.01))                                     OUTP 850
 86:          IIBK=(IFLG-1)*97+(IX+1)                                    OUTP 860
 87:          WRITE(4'IIBK) ((C(M1,K,L),K=2,KY),L=1,N3)                  OUTP 870
 88:          II=II+1                                                    OUTP 880
 89:          IF(X.EQ.0.0) III=0                                         OUTP 890
 90:          IF(X.EQ.0.0) GO TO 15                                      OUTP 900
 91:          AII=FLOAT(III)                                             OUTP 910
 92:          AII1=AII-X/PRDEL                                           OUTP 920
 93:          III=IFIX(AII1*100.)                                        OUTP 930
 94:          IF(III.EQ.0) GO TO 65                                      OUTP 940
 95:          GO TO 800                                                  OUTP 950
 96:       65 CONTINUE                                                   OUTP 960
 97:          III=III+1                                                  OUTP 970
 98:          IF(IFLG.EQ.1.AND.NSRCS.EQ.1) IIII=IIII+1                   OUTP 980
 99:          IIX=IFIX(X/(PRDEL-.01))                                    OUTP 990
100:          IF(IFLG.EQ.NSRCS) GO TO 80                                 OUTP1000
101:          DO 90 J=2,M1                                               OUTP1010
102:          IBLK=J+(IFLG-1)*49*15+IIX*15                               OUTP1020
103:       90 WRITE(2'IBLK) ((C(J,K,L),K=2,KY),L=1,N3)                   OUTP1030
104:          IHL(IFLG,IIX+1)=IHLF                                       OUTP1040
105:          GO TO 800                                                  OUTP1050
106:       80 CALL AVG(C,IIX,IFLAG)                                      OUTP1060
107:          IF(IIX.EQ.1.AND.NSRCS.EQ.1) GO TO 800                      OUTP1070
```

```
108:          IF(IIX.EQ.1) GO TO 74                                    OUTP1080
109:          DO 67 J=2,N1                                             OUTP1090
110:          DO 67 K=2,KY                                             OUTP1100
111:          DO 67 L=1,N3                                             OUTP1110
112:       67 CC(IFLG,J,K,L)=C(J,K,L)                                  OUTP1120
113:          IF(X.EQ.0.0) GO TO 800                                   OUTP1130
114:          T=X-2.*PPDEL                                             OUTP1140
115:          IHL(IFLG,IIX+1)=IHLF                                     OUTP1150
116:          IF(NSRCS.EQ.1) GO TO 18                                  OUTP1160
117:       74 IIFLG=IFLG                                               OUTP1170
118:       78 IIFLG=IIFLG-1                                            OUTP1180
119:          IF(IIFLG.EQ.0) GO TO 18                                  OUTP1190
120:          DO 75 J=2,N1                                             OUTP1200
121:          IPLI=J+(IIFLG-1)*49*15+IIX*15                            OUTP1210
122:       75 READ(2'IPLI) ((C(J,K,L),K=2,KY),L=1,N3)                  OUTP1220
123:          CALL AVG(C,IIX,IIFLG)                                    OUTP1230
124:          IF(IIX.EQ.1.AND.IIFLG.EQ.1) GO TO 800                    OUTP1240
125:          DO 76 J=2,N1                                             OUTP1250
126:          DO 76 K=2,KY                                             OUTP1260
127:          DO 76 L=1,N3                                             OUTP1270
128:       76 CC(IIFLG,J,K,L)=C(J,K,L)                                 OUTP1280
129:          GO TO 78                                                 OUTP1290
130:       15 T=0.                                                     OUTP1300
131:          IIX=0                                                    OUTP1310
132:          DO 91 J=1,NSRCS                                          OUTP1320
133:       91 IHL(J,1)=0                                               OUTP1330
134:          IF(MFLG.EQ.1) GO TO 16                                   OUTP1340
135:          CALL AVG(C,IIX,IFLAG)                                    OUTP1350
136:          III=III+1                                                OUTP1360
137:          GO TO 800                                                OUTP1370
138:       18 CONTINUE                                                 OUTP1380
139:          VAR11=KS(1)                                              OUTP1390
140:          VAR12=LS(1)                                              OUTP1400
141:          CC(1,1,VAR11,VAR12)=CO(1)                                OUTP1410
142:          IF(NSRCS.EQ.1) GO TO 16                                  OUTP1420
143:          DO 17 I=2,NSRCS                                          OUTP1430
```

```
144:          VAR13=I-1                                                        OUTP1440
145:          VAR14=KS(I)                                                      OUTP1450
146:          VAR15=LS(I)                                                      OUTP1460
147:       17 CC(VAR13,N1,VAR14,VAR15)=CC(VAR13,N1,VAR14,VAR15)+CO(I)          OUTP1470
148:       16 WRITE(6,131) T,X,(IHL(J,IIX+1),J=1,NSRCS)                        OUTP1480
149:          WRITE(6,204)                                                     OUTP1490
150:          WRITE(6,210) XXX(1,1),((XXX(J,I),I=2,N1),J=1,NSRCS)              OUTP1500
151:          WRITE(6,215)                                                     OUTP1510
152:          WRITE(6,208)                                                     OUTP1520
153:          L=N3+1                                                           OUTP1530
154:       53 L=L-1                                                            OUTP1540
155:          WRITE(6,205) XZZ(L)                                              OUTP1550
156:          DO 41 K=2,KY                                                     OUTP1560
157:          WRITE(6,134) XYY(K),CC(1,1,K,L),((CC(I,J,K,L),J=2,N1),I=1,NSRCS) OUTP1570
158:       41 CONTINUE                                                         OUTP1580
159:          IF(L.EQ.1) GO TO 40                                              OUTP1590
160:          GO TO 53                                                         OUTP1600
161:       40 CONTINUE                                                         OUTP1610
162:          DO 50 I=1,NSRCS                                                  OUTP1620
163:          DO 50 J=1,N1                                                     OUTP1630
164:          QX(I,J)=0.                                                       OUTP1640
165:          DO 52 K=2,KY                                                     OUTP1650
166:          DO 52 L=1,N3                                                     OUTP1660
167:       52 QX(I,J)=QX(I,J)+CC(I,J,K,L)*U(L)*W2(K)*W3(L)                     OUTP1670
168:          QX(I,J)=QX(I,J)/60000.*H*2.*YMAX                                 OUTP1680
169:       50 CONTINUE                                                         OUTP1690
170:          WRITE(6,220) QX(1,1),((QX(J,I),I=2,N1),J=1,NSRCS)                OUTP1700
171:      900 CONTINUE                                                         OUTP1710
172:  C                                                                        OUTP1720
173:      131 FORMAT(8(/),30X,'THETA =',F6.2,' MIN',/,30X,'OMEGA =',F6.2,' MIN',OUTP1730
174:         110X,'IHLF =',3I3)                                                OUTP1740
175:      134 FORMAT(1X,'Y=',F6.1,' M ',15F8.2)                                OUTP1750
176:      204 FORMAT(//,30X,'X DIRECTION (METERS)',/)                          OUTP1760
177:      205 FORMAT(//,5X,'Z DIRECTION =',F10.1,' M',//)                      OUTP1770
178:      208 FORMAT(35X,'**********************')                            OUTP1780
179:      210 FORMAT(11X,F8.1,1X,14F8.1)                                       OUTP1790
```

```
180:      215 FORMAT(//,38X,'CONCENTRATION(MG/CU.M)')                    OUTP1800
181:      220 FORMAT(4(/),1X,'QX(GR/SEC)=',1PE9.2)                       OUTP1810
182:          RETURN                                                     OUTP1820
183:          END                                                        OUTP1830
```

```
      SUBROUTINE ZERO(C)                                                ZERO  10
C                                                                       ZERO  20
C                                                                       ZERO  30
C  THIS SUBROUTINE CLEANS THE OUTPUT OF THE MODEL                       ZERO  40
C                                                                       ZERO  50
C                                                                       ZERO  60
      DIMENSION C(15,15,15)                                             ZERO  70
      COMMON /BLK1/ A1(15,15),A2(15,15),A3(15,15),P1(15,15),P2(15,15),  ZERO  80
     1P3(15,15),R1(15),P3(15),P5(15),R4(15),R3G1(15),R3G2(15),APA1(15), ZERO  90
     2P36I(15,15),Q(700),U(15),V(15),XXX(3,15),XYY(15),XZZ(15),XMAX(3), ZERO 100
     3YMAX,H,AK,TCH,P,KS(3),LS(3),C0(3),NX,NY,NZ,N1,N2,N3,KX,KY,KZ,     ZERO 110
     4W1(15),W2(15),W3(15),NSRCS,IFLG, IFLG,CC(3,15,15,15),PRDEL,PR4T3, ZERO 120
     5INVRS                                                             ZERO 130
      J=2                                                               ZERO 140
   55 K=KS(IFLG)                                                        ZERO 150
      L=LS(IFLG)                                                        ZERO 160
      IF(C(J,K,L).LE.0.) GO TO 10                                       ZERO 170
   12 L=L+1                                                             ZERO 180
      IF(L.GT.N3) GO TO 14                                              ZERO 190
      IF(C(J,K,L).LE.0.) GO TO 20                                       ZERO 200
      GO TO 12                                                          ZERO 210
   14 L=LS(IFLG)                                                        ZERO 220
   15 L=L-1                                                             ZERO 230
      IF(L.LT.1) GO TO 30                                               ZERO 240
      IF(C(J,K,L).LE.0.) GO TO 25                                       ZERO 250
      GO TO 15                                                          ZERO 260
   20 DO 21 I=L,N3                                                      ZERO 270
   21 C(J,K,I)=0.                                                       ZERO 280
      GO TO 14                                                          ZERO 290
   25 C(J,K,L)=0.                                                       ZERO 300
      L=L-1                                                             ZERO 310
      IF(L.EQ.0) GO TO 30                                               ZERO 320
      GO TO 25                                                          ZERO 330
   30 L=LS(IFLG)                                                        ZERO 340
      K=KS(IFLG)                                                        ZERO 350
```

```
      33 L=LS(IFLG)                                                     ZERO 360
         K=K+1                                                          ZERO 370
         IYD=1                                                          ZERO 380
         IF(K.EQ.N2) GO TO 32                                           ZERO 390
      32 IF(C(J,K,L).LE.0.) GO TO 35                                    ZERO 400
         GO TO 37                                                       ZERO 410
      35 DO 36 I=1,N3                                                   ZERO 420
      36 C(J,K,I)=0.                                                    ZERO 430
         IF(IYD.EQ.1) GO TO 85                                          ZERO 440
         GO TO 86                                                       ZERO 450
      85 DO 80 I=K,KY                                                   ZERO 460
      80 C(J,I,L)=0.                                                    ZERO 470
         GO TO 87                                                       ZERO 480
      86 KIND=K                                                         ZERO 490
      88 C(J,KIND,L)=0.                                                 ZERO 500
         IF(KIND.EQ.1) GO TO 87                                         ZERO 510
         KIND=KIND-1                                                    ZERO 520
         GO TO 88                                                       ZERO 530
      87 CONTINUE                                                       ZERO 540
         IF(IYD.EQ.1) GO TO 33                                          ZERO 550
         GO TO 51                                                       ZERO 560
      37 L=L+1                                                          ZERO 570
         IF(L.GT.N3) GO TO 38                                           ZERO 580
         IF(C(J,K,L).LE.0.) GO TO 39                                    ZERO 590
         GO TO 37                                                       ZERO 600
      39 DO 40 I=L,N3                                                   ZERO 610
      40 C(J,K,I)=0.                                                    ZERO 620
      38 L=LS(IFLG)                                                     ZERO 630
      68 L=L-1                                                          ZERO 640
         IF(L.GE.1) GO TO 63                                            ZERO 650
         IF(IYD.EQ.1) GO TO 33                                          ZERO 660
         IF(IYD.EQ.2) GO TO 51                                          ZERO 670
      63 IF(C(J,K,L).LE.0.) GO TO 42                                    ZERO 680
         GO TO 68                                                       ZERO 690
      42 C(J,K,L)=0.                                                    ZERO 700
         L=L-1                                                          ZERO 710
```

```
72:          IF(L.GE.1) GO TO 42                                    ZERO 720
73:          IF(IYD.EQ.1) GO TO 33                                  ZERO 730
74:          IF(IYD.EQ.2) GO TO 51                                  ZERO 740
75:       32 L=LS(IFLG)                                             ZERO 750
76:          K=KS(IFLG)                                             ZERO 760
77:       51 L=LS(IFLG)                                             ZERO 770
78:          K=K-1                                                  ZERO 780
79:          IYD=2                                                  ZERO 790
80:          IF(K.EQ.1) GO TO 50                                    ZERO 800
81:          GO TO 52                                               ZERO 810
82:       50 J=J+1                                                  ZERO 820
83:          IF(J.GT.N1) GO TO 60                                   ZERO 830
84:          GO TO 55                                               ZERO 840
85:       10 DO 58 I=J,N1                                           ZERO 850
86:          DO 58 K=2,KY                                           ZERO 860
87:          DO 58 L=1,N3                                           ZERO 870
88:       58 C(I,K,L)=0.                                            ZERO 880
89:       60 CONTINUE                                               ZERO 890
90:          RETURN                                                 ZERO 900
91:          END                                                    ZERO 910
```

```
      SUBROUTINE AVG(C,II,IFLAG)                                        AVG   10
C                                                                       AVG   20
C                                                                       AVG   30
C   THIS SUBROUTINE COMPUTES THE AVERAGE CONCENTRATIONS (AVERAGING      AVG   40
C   TIME = 2*PRDEL)                                                     AVG   50
C                                                                       AVG   60
C                                                                       AVG   70
      DIMENSION C(15,15,15),D(15,15,15)                                 AVG   80
      COMMON /PLK1/ A1(15,15),A2(15,15),A3(15,15),B1(15,15),B2(15,15),  AVG   90
     1B3(15,15),R1(15),R3(15),R5(15),R6(15),R3B1(15),R3B2(15),APA1(15), AVG  100
     2B3B1(15,15),C(700),U(15),V(15),XXX(3,15),XYY(15),XZZ(15),XMAX(3), AVG  110
     3YMAX,H,AK,TCH,P,KS(3),IS(3),CO(3),NX,NY,NZ,N1,N2,N3,KX,KY,KZ,      AVG  120
     4W1(15),W2(15),W3(15),NSRCS,IFLG,MFLG,CC(3,15,15,15),PRDEL,PRMTS,  AVG  130
     5INVRS                                                             AVG  140
      IF(II.GT.2) GO TO 90                                              AVG  150
      M=II+1                                                            AVG  160
      DO 10 J=2,N1                                                      AVG  170
      IRLK=J+(IFLAG-1)*15+(M-1)*45                                      AVG  180
   10 WRITE(3'IRLK) ((C(J,K,L),K=2,KY),L=1,N3)                          AVG  190
      IF(II.EQ.2) GO TO 80                                              AVG  200
      RETURN                                                            AVG  210
   90 M=2                                                               AVG  220
      DO 15 J=2,N1                                                      AVG  230
      IRLK=J+(IFLAG-1)*15+(M-1)*45                                      AVG  240
   15 READ(3'IRLK) ((D(J,K,L),K=2,KY),L=1,N3)                           AVG  250
      M=1                                                               AVG  260
      DO 25 J=2,N1                                                      AVG  270
      IRLK=J+(IFLAG-1)*15+(M-1)*45                                      AVG  280
   25 WRITE(3'IRLK) ((D(J,K,L),K=2,KY),L=1,N3)                          AVG  290
      M=3                                                               AVG  300
      DO 35 J=2,N1                                                      AVG  310
      IRLK=J+(IFLAG-1)*15+(M-1)*45                                      AVG  320
   35 READ(3'IRLK) ((D(J,K,L),K=2,KY),L=1,N3)                           AVG  330
      M=2                                                               AVG  340
      DO 45 J=2,N1                                                      AVG  350
```

```
36:          IBLK=J+(IFLAG-1)*15+(M-1)*45                              AV  360
37:       45 WRITE(3'IBLK) ((D(J,K,L),K=2,KY),L=1,N3)                  AV  370
38:          M=3                                                       AVG 380
39:          DO 55 J=2,N1                                              AVG 390
40:          IBLK=J+(IFLAG-1)*15+(M-1)*45                              AVG 400
41:       55 WRITE(3'IBLK) ((C(J,K,L),K=2,KY),L=1,N3)                  AVG 410
42:       80 CONTINUE                                                  AVG 420
43:          M=1                                                       AVG 430
44:          DO 70 J=2,N1                                              AVG 440
45:          IBLK=J+(IFLAG-1)*15+(M-1)*45                              AVG 450
46:       70 READ(3'IBLK) ((C(J,K,L),K=2,KY),L=1,N3)                   AVG 460
47:          M=2                                                       AVG 470
48:          DO 71 J=2,N1                                              AVG 480
49:          IBLK=J+(IFLAG-1)*15+(M-1)*45                              AVG 490
50:       71 READ(3'IBLK) ((D(J,K,L),K=2,KY),L=1,N3)                   AVG 500
51:          DO 72 J=2,N1                                              AVG 510
52:          DO 72 K=2,KY                                              AVG 520
53:          DO 72 L=1,N3                                              AVG 530
54:       72 C(J,K,L)=C(J,K,L)+D(J,K,L)                                AVG 540
55:          M=3                                                       AVG 550
56:          DO 73 J=2,N1                                              AVG 560
57:          IBLK=J+(IFLAG-1)*15+(M-1)*45                              AVG 570
58:       73 READ(3'IBLK) ((D(J,K,L),K=2,KY),L=1,N3)                   AVG 580
59:          DO 74 J=2,N1                                              AVG 590
60:          DO 74 K=2,KY                                              AVG 600
61:          DO 74 L=1,N3                                              AVG 610
62:       74 C(J,K,L)=(C(J,K,L)+D(J,K,L))/3.                           AVG 620
63:          RETURN                                                    AVG 630
64:          END                                                       AVG 640
```

```
      SUBROUTINE RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)                RKGS  10
C                                                                        RKGS  20
C                                                                        RKGS  30
C  THIS SUBROUTINE SOLVES A SYSTEM OF FIRST ORDER ORDINARY DIFFERENTIAL  RKGS  40
C  EQUATIONS WITH GIVEN INITIAL CONDITIONS                               RKGS  50
C                                                                        RKGS  60
C                                                                        RKGS  70
C     PRMT        - AN INPUT OUTPUT VECTOR WITH DIMENSION GREATER OR     RKGS  80
C                   EQUAL TO 5                                           RKGS  90
C     PRMT(1)     - LOWER BOUND OF THE INTERVAL                          RKGS 100
C     PRMT(2)     - UPPER BOUND OF THE INTERVAL                          RKGS 110
C     PRMT(3)     - INITIAL INCREMENT OF THE INDEPENDENT VARIABLE        RKGS 120
C     PRMT(4)     - UPPER ERROR BOUND                                    RKGS 130
C     PRMT(5)     - NO INPUT PARAMETER. IT IS 0 UNLESS THE USER WANTS TO RKGS 140
C                   TERMINATE RKGS AT ANY OUTPUT POINT                   RKGS 150
C     DERY        - INPUT VECTOR OF ERROR WEIGHTS. LATER ON IS THE VECTOR RKGS 160
C                   OF DERIVATIVES                                       RKGS 170
C     NDIM        - THE NUMBER OF EQUATIONS IN THE SYSTEM                RKGS 180
C     IHLF        - THE NUMBER OF BISECTIONS OF THE INITIAL INCREMENT     RKGS 190
C     AUX         - AN AUXILIARY STORAGE ARRAY (8 ROWS AND NDIM COLUMNS) RKGS 200
C                                                                        RKGS 210
C                                                                        RKGS 220
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(1)             RKGS 230
      DO 1 I=1,NDIM                                                      RKGS 240
    1 AUX(8,I)=.06666667*DERY(I)                                         RKGS 250
      X=PRMT(1)                                                          RKGS 260
      XEND=PRMT(2)                                                       RKGS 270
      H=PRMT(3)                                                          RKGS 280
      PRMT(5)=0.                                                         RKGS 290
      CALL FCT(X,Y,DERY)                                                 RKGS 300
C                                                                        RKGS 310
C  ERROR TEST                                                            RKGS 320
C                                                                        RKGS 330
      IF(H*(XEND-X))38,37,2                                              RKGS 340
C                                                                        RKGS 350
```

```
C  PREPARATIONS FOR RUNGE-KUTTA METHOD                              RKGS  360
C                                                                   RKGS  370
     2 A(1)=.5                                                      RKGS  380
       A(2)=.2928932                                                RKGS  390
       A(3)=1.707107                                                RKGS  400
       A(4)=.1666667                                                RKGS  410
       B(1)=2.                                                      RKGS  420
       B(2)=1.                                                      RKGS  430
       B(3)=1.                                                      RKGS  440
       B(4)=2.                                                      RKGS  450
       C(1)=.5                                                      RKGS  460
       C(2)=.2928932                                                RKGS  470
       C(3)=1.707107                                                RKGS  480
       C(4)=.5                                                      RKGS  490
C                                                                   RKGS  500
C  PREPARATIONS OF FIRST RUNGE-KUTTA STEP                           RKGS  510
C                                                                   RKGS  520
       DO 3 I=1,NDIM                                                RKGS  530
       AUX(1,I)=Y(I)                                                RKGS  540
       AUX(2,I)=DERY(I)                                             RKGS  550
       AUX(3,I)=0.                                                  RKGS  560
     3 AUX(6,I)=0.                                                  RKGS  570
       IREC=0                                                       RKGS  580
       H=H+H                                                        RKGS  590
       IHLF=-1                                                      RKGS  600
       ISTEP=0                                                      RKGS  610
       IEND=0                                                       RKGS  620
C                                                                   RKGS  630
C  START OF A RUNGE-KUTTA STEP                                     RKGS  640
C                                                                   RKGS  650
     4 IF((X+H-XEND)*H)7,6,5                                        RKGS  660
     5 H=XEND-X                                                     RKGS  670
     6 IEND=1                                                       RKGS  680
C                                                                   RKGS  690
C  RECORDING OF INITIAL VALUES OF THIS STEP                         RKGS  700
C                                                                   RKGS  710
```

```
      7 CALL OUTP(X,Y,DERY,IREC,NLIM,PRMT)                              RKGS 720
        IF(PRMT(5))40,8,40                                              RKGS 730
      8 ITEST=0                                                         RKGS 740
      9 ISTEP=ISTEP+1                                                   RKGS 750
C                                                                       RKGS 760
C   START OF INNERMOST RUNGE-KUTTA LOOP                                 RKGS 770
C                                                                       RKGS 780
        J=1                                                             RKGS 790
     10 AJ=A(J)                                                         RKGS 800
        BJ=B(J)                                                         RKGS 810
        CJ=C(J)                                                         RKGS 820
        DO 11 I=1,NDIM                                                  RKGS 830
        R1=H*DERY(I)                                                    RKGS 840
        R2=AJ*(R1-BJ*AUX(3,I))                                          RKGS 850
        Y(I)=Y(I)+R2                                                    RKGS 860
        R2=R2+R2+R2                                                     RKGS 870
     11 AUX(3,I)=AUX(3,I)+R2-CJ*R1                                      RKGS 880
        IF(J-4)12,15,15                                                 RKGS 890
     12 J=J+1                                                           RKGS 900
        IF(J-3)13,14,13                                                 RKGS 910
     13 X=X+.5*H                                                        RKGS 920
     14 CALL FCT(X,Y,DERY)                                              RKGS 930
        GOTO 10                                                         RKGS 940
C                                                                       RKGS 950
C   TEST OF ACCURACY                                                    RKGS 960
C                                                                       RKGS 970
     15 IF(ITEST)16,16,20                                               RKGS 980
C                                                                       RKGS 990
C   IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING OF ACCURACY     RKGS1000
C                                                                       RKGS1010
     16 DO 17 I=1,NDIM                                                  RKGS1020
     17 AUX(4,I)=Y(I)                                                   RKGS1030
        ITEST=1                                                         RKGS1040
        ISTEP=ISTEP+ISTEP-2                                             RKGS1050
     18 IHLF=IHLF+1                                                     RKGS1060
        X=X-H                                                           RKGS1070
```

```
      H=.5*H                                                            RKGS1080
      DO 19 I=1,NDIM                                                    RKGS1090
      Y(I)=AUX(1,I)                                                     RKGS1100
      DERY(I)=AUX(2,I)                                                  RKGS1110
   19 AUX(5,I)=AUX(3,I)                                                 RKGS1120
      GOTO 9                                                            RKGS1130
C                                                                       RKGS1140
C  IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE                      RKGS1150
C                                                                       RKGS1160
   20 IMOD=ISTEP/2                                                      RKGS1170
      IF(ISTEP-IMOD-IMOD)21,23,21                                       RKGS1180
   21 CALL FCT(X,Y,DERY)                                                RKGS1190
      DO 22 I=1,NDIM                                                    RKGS1200
      AUX(5,I)=Y(I)                                                     RKGS1210
   22 AUX(7,I)=DERY(I)                                                  RKGS1220
      GOTO 9                                                            RKGS1230
C                                                                       RKGS1240
C  COMPUTATION OF TEST VALUE DELT                                       RKGS1250
C                                                                       RKGS1260
   23 DELT=0.                                                           RKGS1270
      DO 24 I=1,NDIM                                                    RKGS1280
   24 DELT=DELT+AUX(8,I)*ABS(AUX(4,I)-Y(I))                             RKGS1290
      IF(DELT-PRMT(4))28,28,25                                          RKGS1300
C                                                                       RKGS1310
C  ERROR IS TOO GREAT                                                   RKGS1320
C                                                                       RKGS1330
   25 IF(IHLF-10)26,36,36                                               RKGS1340
   26 DO 27 I=1,NDIM                                                    RKGS1350
   27 AUX(4,I)=AUX(5,I)                                                 RKGS1360
      ISTEP=ISTEP+ISTEP-4                                               RKGS1370
      X=X-H                                                             RKGS1380
      IEND=0                                                            RKGS1390
      GOTO 18                                                           RKGS1400
C                                                                       RKGS1410
C  RESULT VALUES ARE GOOD                                               RKGS1420
C                                                                       RKGS1430
```

```
144:      28 CALL FCT(X,Y,DERY)                                          RKGS1440
145:         DO 29 I=1,NDIM                                              RKGS1450
146:         AUX(1,I)=Y(I)                                               RKGS1460
147:         AUX(2,I)=DERY(I)                                            RKGS1470
148:         AUX(3,I)=AUX(6,I)                                           RKGS1480
149:         Y(I)=AUX(5,I)                                               RKGS1490
150:      29 DERY(I)=AUX(7,I)                                            RKGS1500
151:         CALL OUTP(X-H,Y,DERY,IHLF,NDIM,PRMT)                        RKGS1510
152:         IF(PRMT(5))40,30,40                                         RKGS1520
153:      30 DO 31 I=1,NDIM                                              RKGS1530
154:         Y(I)=AUX(1,I)                                               RKGS1540
155:      31 DERY(I)=AUX(2,I)                                            RKGS1550
156:         IPFC=IHLF                                                   RKGS1560
157:         IF(IEND)32,32,39                                            RKGS1570
158:   C                                                                 RKGS1580
159:   C  INCREMENT GETS DOUBLED                                         RKGS1590
160:   C                                                                 RKGS1600
161:      32 IHLF=IHLF-1                                                 RKGS1610
162:         ISTEP=ISTEP/2                                               RKGS1620
163:         H=H+H                                                       RKGS1630
164:         IF(IHLF)4,33,33                                             RKGS1640
165:      33 IMOD=ISTEP/2                                                RKGS1650
166:         IF(ISTEP-IMOD-IMOD)4,34,4                                   RKGS1660
167:      34 IF(DELT-.02*PRMT(4))35,35,4                                 RKGS1670
168:      35 IHLF=IHLF-1                                                 RKGS1680
169:         ISTEP=ISTEP/2                                               RKGS1690
170:         H=H+H                                                       RKGS1700
171:          GOTO 4                                                     RKGS1710
172:   C                                                                 RKGS1720
173:   C  RETURNS TO CALLING PROGRAM                                     RKGS1730
174:   C                                                                 RKGS1740
175:      36 IHLF=11                                                     RKGS1750
176:         CALL FCT(X,Y,DERY)                                          RKGS1760
177:         GOTO 39                                                     RKGS1770
178:      37 IHLF=12                                                     RKGS1780
179:         GOTO 39                                                     RKGS1790
```

```
180:      38 IHLF=13                                                    RKGS1900
181:      39 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                         RKGS1910
182:      40 RETURN                                                     RKGS1920
183:         END                                                        RKGS1930
```

APPENDIX B

INPUT DATA REQUIRED

As examples, the input information for the hypothetical cases 8 and 10 are given next.

INPUT DATA (Case #8)

TINIT = 0.0 ENDS = 90.0 MIN PRMT(3) = 2.5C MIN PRMT(4) = 1.CCCCC

NUMBER OF SOURCES = 1

PRDEL = 5.CO MIN

NX = 6 NY = 7 NZ = 7

YMAX = 7CO.0 M H = 505.CO M

KS = 5 LS = 4 CC = 35.45 MG/CU.M XMAX = 10000.0 M

STABILITY CLASS = 4 INVRS = 1 ALPHA = 2.CC AK = C.58E-C4 1/MIN

UST = 3CC.CC M/MIN LGR = 30.CO M/MIN AM = 0.250 TCH = 15.0 MIN P = 0.05

INPUT DATA (Case #10)

TINIT = 0.C ENDS = 90.0 MIN PRMT(3) = 2.50 MIN PRMT(4) = 1.CCCCC

NUMBER OF SOURCES = 2

PRDEL = 5.CO MIN

NX = 6 NY = 7 NZ = 7

YMAX = 7CC.0 M H = 505.CO M

KS = 5 LS = 4 CO = 35.45 MG/CU.M XMAX = 1CCCO.0 M

KS = 4 LS = 5 CO = 21.27 MG/CU.M XMAX = 8CCO.C M

STABILITY CLASS = 4 INVRS = 1 ALPHA = 2.CO AK = C.58E-C4 1/MIN

UST = 3CO.CC M/MIN LGR = 30.CO M/MIN AM = 0.250 TCH = 15.C MIN P = 0.0

APPENDIX C

NOMENCLATURE

a	Constant in equation (4.8)
a_i	Parameters defined by equation (4.2)
a_{ij}	Parameters defined by equation (4.41)
$\underline{\underline{A}}$	Matrix defined by equation (4.19)
AM	Represents the exponent m
b	Constant in equation (4.29)
$\underline{\underline{B}}$	Matrix defined by equation (4.20)
c	Constant in equation (4.29)
c_j	Coefficients in equation (4.3)
C_i	Instantaneous concentration of species i, mg/m^3
C_B	Background concentration
$C_o(i)$	Concentration at i^{th} source
d_i	Coefficients defined by equation (4.11)
d_{ij}	Coefficients defined by equation (4.42)
D_i	Molecular diffusivity of species i, m^2/min
D'	Eddy diffusivity tensor used in equation (3.1)
e_i	Constants defined by equation (4.43)
f_j	Constants defined by equation (4.50)
G_i	Constant given by equation (4.9)

G_i^*	Constant in equation (4.33)
H	Maximum height above terrain (in some cases refers to the elevation of the inversion base)
INVRS	Constant used in equation (4.105)
ISTB	Stability class (1 very unstable, 6 very stable)
(JS,KS,LS)	(x,y,z) coordinate position of a point source
k	Reaction rate constant, min^{-1}
k_o	Von Karman's constant
K	Turbulent diffusivity, m^2/min
ℓ	Height defined by equation (3.11)
L	Effective emission height, m
m	Exponent in equation (4.65)
N	Number of interior collocation points
N_j	j^{th} independent Gaussian white noise
NSRCS	Number of sources
p	Exponent in equation (3.10)
P	Constant in equation (4.67)
P_o	First orthogonal polynomial
P_i	i^{th} orthogonal polynomial
P_j	Power spectral density of the j^{th} white noise
PRMT(3)	Initial step size of integration
PRMT(4)	Upper error bound in "RKGS"
Q	Source emission rate, $mg/m^3 min$
Q(i)	Strength of i^{th} continuous point source, kg/s
$\bar{\bar{Q}}$	Matrix used in orthogonal collocation theory
Q_x	Mass rate through y-z plane at x = constant, kg/s

$Q(x,t/x^*,t^*)$	Transition probability density function
$\bar{\bar{R}}$	Matrix used in orthogonal collocation theory
R_i	Rate of generation of species i
s	Number of species
S(x,t)	Spatial-temporal distribution of particle sources
t	Time, min
$\bar{\bar{T}}$	Matrix used in orthogonal collocation theory
TCH	Parameter in equation (4.67)
u	Velocity in x-direction, m/min
u	Variable in equation (4.31)
u_j	j^{th} component of fluid velocity, m/min
$u*$	Friction velocity
UGR	Mean wind velocity in the x-direction at ground level
UST	Geostrophic wind speed, m/min
v	Velocity in y-direction, m/min
v*	Pseudo-velocity defined by equation (3.1)
w	Velocity in z-direction, m/min
w(x)	Weighting function
W_j	Quadrature weights
x	Cartesian coordinate in mean wind direction
x	Refers to independent variable in orthogonal collocation theory
x_j	Collocation points
x_{max}	Maximum distance in the x-direction

y	Cartesian coordinate in horizontal direction
y	Refers to dependent variable in orthogonal collocation theory
y_{max}	Maximum distance in the y-direction
z	Cartesian coordinate in vertical direction
z_o	Characteristic surface roughness length
z_1	Reference height

Greek Symbols

α	Constant in equation (4.63)
α	Exponent in equation (4.5)
∇	Gradient vector
∇^2	Laplacian
β	Exponent in equation (4.5)
Γ	Gamma function
δ	Test value used in "RKGS"
δ_{ij}	Kronecker delta function
Δ	Knee height, m
ζ	Function that represents K_z
η	Function that represents v
θ	Time between the pollutant release and the initiation of the averaging time, min
ξ	Function that represents K_y
σ	Standard deviation
$\phi(x,y)$	Function of the independent variables x and y, given by equation (4.41)

ψ Function that represents u

Ω End of the averaging time, min

Superscripts

' Denotes the fluctuating component when used in a concentration or velocity variable

$\bar{}$ Denotes the mean value when used on a velocity variable

* Refers to shifted polynomials

= Refers to a matrix

Subscripts

i i^{th} species

i Index in collocation equations

i Index used in orthogonal collocation theory

j j^{th} direction in Cartesian coordinates

j Index used in orthogonal collocation theory

j Represents the x-direction in collocation equations

k Represents the y-direction in collocation equations

ℓ Represents the z-direction in collocation equations

n Index used in orthogonal collocation theory

s Denotes ground level

x Refers to x coordinate direction

y Refers to y coordinate direction

z Refers to z coordinate direction

~ Denotes a vector quantity

Brackets

< > Denotes ensemble averages